

DOKUZ EYLÜL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

**THERMAL CHARACTERIZATION OF
SAND-BENTONITE MIXTURES WITH
BORON ADDITIVES**

by
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July, 2019
İZMİR

THERMAL CHARACTERIZATION OF SAND- BENTONITE MIXTURES WITH BORON ADDITIVES

**A Thesis Submitted to the
Graduate School of Natural and Applied Sciences of Dokuz Eylül University
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in Civil Engineering, Geotechnical Program**

**by
Mesut Şahin IRGAT**

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İZMİR**

M.Sc THESIS EXAMINATION RESULT FORM

We have read the thesis entitled “**THERMAL CHARACTERIZATION OF SAND-BENTONITE MIXTURES WITH BORON ADDITIVES**” completed by **MESUT ŞAHİN IRGAT** under supervision of **PROF. DR. YELİZ YÜKSELEN AKSOY** and we certify that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.



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THERMAL CHARACTERIZATION OF SAND- BENTONITE MIXTURES WITH BORON ADDITIVES

ABSTRACT

Due to increasing energy demand in the world, an increase in the diversity of energy structures is observed. In recent years, there has been a focus on energy structures such as energy piles, geothermal energy plants and nuclear power stations. These thermo-active structures cause temperature increases in soil. Because of these temperature differences, changes in soil parameters occur and as a result of these changes, the mechanical, hydraulic and thermal properties of the soil do not meet the expected performance limits and causing damage to energy structures. Soil thermal conductivity coefficient, heat diffusion coefficient and heat storage capacities are the parameters controlling the heat transfer mechanism in soils. Therefore, in this thesis, thermal conductivity coefficients of boron added sand-bentonite mixtures and usability of these mixtures as a buffer material in the disposal repositories of high grade radioactive wastes (HLW) were investigated. In addition, the effects of thermal conductivity coefficient, volumetric heat capacity and heat diffusion coefficient values on heat conduction, which have a role in heat transfer mechanism, have been investigated. Instead of bentonite material used as a buffer around canister where waste is stored in nuclear waste repositories, boron added sand-bentonite mixtures were used in this thesis, single and double layer structures were designed separately and analyzed with the help of two different computer program using finite element method. According to the results obtained from this study; the lowest and highest thermal conductivity values were obtained in mixtures containing five percent and fifteen percent tincal, respectively. The maximum temperature in the buffer layer was calculated seventeen degrees lower than that of bentonite alone.

Keywords: Boron, nuclear waste repositories, thermal conductivity, bentonite buffer, Ansys, Code_Bright, thermal analysis

BOR KATKILI KUM-BENTONİT KARIŞIMLARININ TERMAL KARAKTERİZASYONU

ÖZ

Dünyada artan enerji gereksinimi nedeni ile enerji yapılarının çeşitliliğinde artış gözlemlenmektedir. Son yıllarda enerji kazıkları, jeotermal enerji tesisleri ve nükleer enerji santralleri üzerine yoğunlaşma olmuştur. Termal olarak aktif olan bu yapılar zemin içerisinde sıcaklık farklarının oluşmasına neden olmaktadır. Bu sıcaklık farklarından ötürü zemin parametrelerinde değişimler meydana gelmekte olup bu değişimler neticesinde zeminlerin mekanik, hidrolik ve termal özelliklerinin beklenen performans limitlerini karşılayamaması enerji yapılarında hasara neden olabilmektedir. Zeminlerin termal iletkenlik katsayıları, ısı yayılım hızları ve depolama kapasiteleri zeminlerde ısı transfer mekanizmasını kontrol eden parametrelerdir. Bu nedenle bu çalışmada bor katkılı kum-bentonit karışımlarının termal iletkenlik katsayıları ile bu karışımların yüksek dereceli radyoaktif atıkların bertarafı aşamasında tampon malzemesi olarak kullanılabilirliği ısısal yönden araştırılmıştır. Bununla beraber ısı transferi mekanizmasında rol oynayan malzeme özelliklerinden termal iletkenlik katsayısı, ısı depolama kapasitesi ve ısı yayılım katsayısı değerlerinin ısı enerjisi iletiminde etkileri irdelenmiştir. Nükleer atık depo sahalarında atığın depolandığı çelik varil etrafında tampon görevinde kullanılan bentonite malzemesi yerine, bu tez çalışmada bor katkılı kum-bentonit karışımları kullanılarak tek ve çift tabakalı yapılar dizayn edilmiş ve iki farklı sonlu elemanlar metodo kullanan paket program yardımı ile analiz edilmiştir. Bu çalışmadan elde edilen sonuçlara göre; en düşük ve en yüksek termal iletkenlik değerleri sırasıyla yüzde beş ve yüzde onbeş tinkal içeren karışımlarda elde edilmiştir. Tinkal katkılı karışımlar kullanılarak dizayn edilen modelde tampon tabakası içerisindeki maksimum sıcaklık değeri, bentonit kullanılmasına nazaran on yedi derece daha düşük hesaplanmıştır.

Anahtar kelimeler: Bor, nükleer atık depo sahası, termal iletkenlik, bentonit tampon, Ansys, Code_Bright, termal analiz

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CHAPTER ONE

INTRODUCTION

In today's societies with developed industries, insufficient energy resources pose a serious energy problem worldwide as a result of the inefficient use of current resources and the increasing human population. There has been a move towards new energy sources because traditional fossil fuels are expensive and their resources have been depleted. It is important that new energy sources be sustainable, environmentally friendly and efficient. Thus, some research areas, such as wind energy, solar energy, geothermal energy and nuclear energy, as well as energy piles, have become important in recent years.

Energy piles cause thermal changes in the soil that they are directly in contact with. In addition to these structures, thermal cycles occur in the soils around heat storage facilities, high-voltage underground cables and CO₂ storage facilities. Therefore, the number of studies about the engineering behavior of soils subject to high amount of heat and thermal cycles has recently increased. These studies have revealed that thermal cycles (heating–cooling) and high amounts of heat cause changes in the engineering properties of soils, such as hydraulic conductivity, volumetric deformation (settlement–swelling), and shear strength. Heat increases in soils may negatively affect engineering behavior. For example, increases in hydraulic conductivity values due to thermal effects in impermeable sand–bentonite barriers used for nuclear waste isolation may cause irreversible environmental pollution. Volumetric deformation or strength loss in the soils around other power structures may harm certain functions of these structures.

It is known that high amounts of heat are released in nuclear waste disposal areas (Abuel-Naga et al., 2006). Heat increases are also observed in the soils around energy piles, heat storage facilities, high-voltage underground pipes, geothermal facilities and similar structures. Heat is released in dumpsites as a result of decomposition of organic compounds and biochemical reactions. This released heat negatively affects the long-

term thermo-hydro-mechanical (THM) behavior of soils used in impermeable layers in dumpsites.

Heat is a type of energy measured in joules. Heat energy is easily lost from energy system compared to other energy types, which in turn results in several problems. Excessive heat energy can seriously damage surrounding buffer in nuclear waste repositories, and if measures are not taken it can be very dangerous – even causing worldwide destruction. Heat energy losses decrease the efficiency of related systems and cause the system to fail to operate at their required performance level. For example, when the pipes carrying hot water to underground geothermal facilities are not properly insulated, hot water passing through the pipes transfer their heat energy to the surrounding soil, which will decrease the temperature of the water inside the pipe and thus, water will not be provided to the geothermal facilities at the desired temperature. Furthermore, increased temperatures in the surrounding soils due to heat transfer can alter the engineering properties of the soil and destroy vegetation cover.

1.1 Background

1.1.1 High-Level Nuclear Waste Repositories

Even if all the energy resources of Turkey are put into service before 2020, it will still not be possible to meet the total energy demand. The construction of nuclear power plants, which is the most important alternative to fossil fuels, is currently an issue in Turkey (Türkiye Elektrik Üretimi ve Dağıtım Şirketi-TEÜD, 1999). In developed countries, the majority of the energy demand is satisfied by nuclear power stations. Nuclear waste produced by nuclear power stations in other countries is disposed in excavated underground geological repositories. They should be properly isolated to avoid them polluting the environment (International Atomic Energy Agency -IAEA, 1990; IAEA, 2003). In terms of the success of nuclear waste storage isolation, it is crucial that materials should be mechanically stable, chemically resistant and have very low hydraulic permeability (IAEA, 2001).

Because bentonite and sand–bentonite mixtures meet the requirements mentioned above, they are used as buffer and filling materials to isolate underground nuclear waste repositories in Sweden, Switzerland, Canada, Germany and France (Pusch, 1994). The purpose in using sand–bentonite as an impermeable barrier is first to get a two-component isolation material by adding bentonite to sand in a specific ratio, and then constructing a resistant and relatively impermeable buffer material by forming the load-carrying skeleton with the sand component and using the bentonite component to form the impermeable barrier to fill the voids in the sand (Mollins et al., 1998). It is necessary for the hydraulic permeability values of compacted clay barriers as a buffer to be at a level of 1×10^{-12} m/s (Kim, Kwon, Sanchez, & Cho, 2011). Westsik et al. (1982) and Radhakrishna et al. (1989) stated that when mixtures of compacted sand–bentonite are used in the isolation of nuclear waste, their hydraulic conductivity values should be 1×10^{-11} m/s or below.

High-level radioactive wastes are the highly radioactive materials produced that arise as a byproduct of nuclear power generation. (United States Nuclear Regulatory Commission, 2017). Spent nuclear fuel is no longer efficient in creating electricity, because its fission process has slowed. However, it is still thermally hot, highly radioactive, and very harmful. Because of their highly radioactive fission products, high-level waste and spent fuel must be handled and stored with care. Since the only way radioactive waste finally becomes harmless is through decay, which for high-level wastes can take 10000 years, the wastes must be stored and finally disposed of in a way that provides adequate protection of the public for a very long time. Because HLW contains relatively high concentrations of both highly radioactive and extremely long-lived radionuclides, special disposal practices are needed. They are solidified, generally in a glass matrix in a process known as vitrification.

In order to dispose of HLW, an international consensus has emerged that deep geological disposal on land is the most appropriate means for isolating such wastes permanently from human environment. Radioactive wastes present no hazard while they remain in a deep underground repository. Because of their depth of burial (several hundreds of metres or more), the possibility of intentional human intrusion is virtually

eliminated. Geological units under consideration are rock salt, argillaceous formations (clays), and a range of crystalline rock formations including granite, welded tuff, basalt, and various metamorphic rock types (OECD Nuclear Energy Agency, 1989).

Because consumed spent fuel in nuclear power plants is radioactive, it releases heat and nuclear radiation to the surroundings during its half-life, depending on the type of radioactive substance in the waste. Many methods have been developed for the disposal of this waste, and presently necessary research and experiments into related projects continues. The most important large-scale experiment is FEBEX (full-scale high-level engineered barriers experiment) and experiments have been carried out for more than 18 years in the Grimsel (Switzerland) area (Antonio Gens, 2019).

Research into the disposal of high level waste (HLW), which has a high amount of radioactivity, continues. In one such study, the waste is placed inside cylindrical canisters made from special materials, as shown in Figure 1.1, and buried inside a rock formation approximately 500 m below ground after wrapping them with a compacted bentonite material.

Their disposal, by placing vertically and horizontally inside the rock (Figure 1.2), has been studied by many scientists in terms of applicability and sustainability. The systems considered for the disposal of HLWs have three basic materials: impermeable host rock, backfill and bentonite. The purposes for using these three materials to dispose of HLWs, and the requirements of dumpsites, are explained by the IAEA (1981).

As the IAEA (1981) report states, the most important reason for using bentonite material surrounding the canister is the hydraulic conductivity and swelling potential properties of the bentonite material. Another important feature of the material that can serve as a buffer is its thermal conductivity value. In other words; the hydraulic conductivity value of the buffer material should be very low and the swelling potential and thermal conductivity values should be very high. The low hydraulic conductivity value is very important for the microorganisms in the underground to pass through the

buffer material and not to carry the radiation, which is generated on the canister surface, to the surface. High thermal conductivity value is very important because it is aimed to minimize the temperature increases that may occur on the canister surface and in bentonite material. It is known that there are some very important limit values in the project planning of storage of HLW type wastes which are given in Figure 1.2.



Figure 1.1 Disposal canister of a Korean reference disposal system (Lee et. al., 2012)

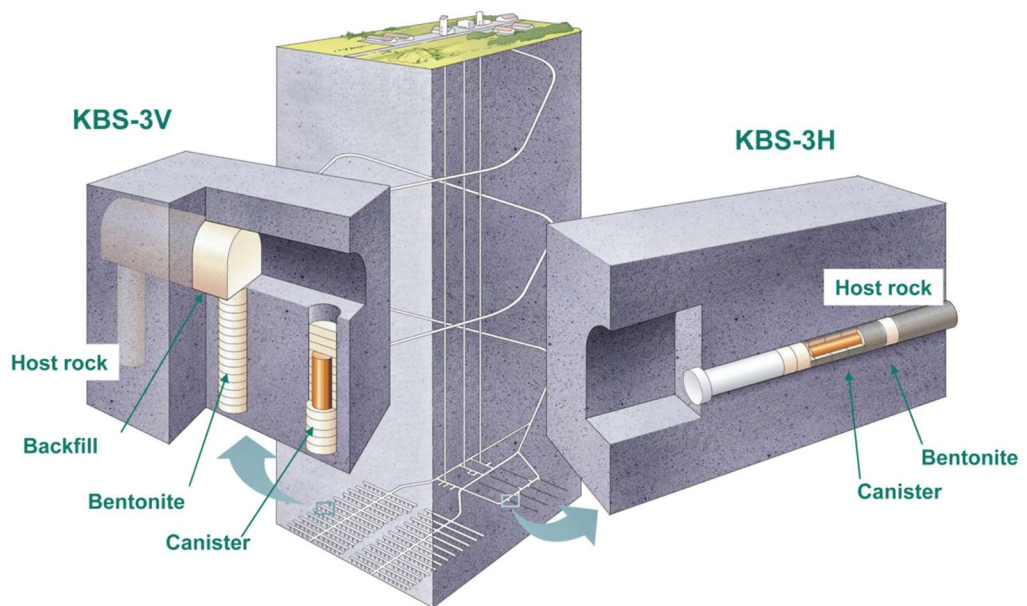


Figure 1.2 Vertical and horizontal spent fuel canister (Posiva, 2019)

The most important design characteristics are that the hydraulic conductivity value of the buffer material is less than 1×10^{-12} m/s and the peak temperature in the buffer layer that contacts the canister surface is below 100°C (Ballarini, Graupner, & Bauer, 2017; Boase & Vandergraaf, 2017; A. Gens, Guimarães, Olivella, & Sánchez, 2010; Antonio Gens & Olivella, 2007; IAEA, 1983; Kim, Kwon, Sanchez, & Cho, 2011; Lee et al., 2012; Sasaki, Ando, Kawamura, & Schneider, 1997). The summary of these design limits are given in Table 1.1.

Table 1.1 Performance Indicators for the Buffer (Kim et al., 2011)

Performance indicator	Criterion	Background
Hydraulic conductivity	$k^{Buffer} < 10^{-12}$ m/s	Limit mass transport to a diffusion-dominated process
Swelling pressure	$P_{swell} > 1$ MPa	Ensure sealing, self-healing capacity
Maximum temperature	$T^{Buffer} < 100^{\circ}\text{C}$	Ensure that the buffer retains its properties for long periods of time
Minimum temperature	$T^{Buffer} > -5^{\circ}\text{C}$	Prevent freezing
Swelling pressure against the canister	$P_{swell} > 0.2$ MPa	Prevent the canister from sinking
Swelling pressure around the canister	$P_{swell} > 2$ MPa	Prevent microbial activity
Density around the canister	$\rho_{Bulk} > 1,650$ kg/m ³	Prevent transport of particles through the buffer
Density around the canister	$\rho_{Bulk} < 2,100$ kg/m ³	Limit shear stresses on the canister due to rock movements

In addition to the limit values given in Table 1.1, the analysis and reasons of designing the canister, buffer, backfill and spent fuel which are used in HLW type nuclear waste repositories are given in Table 1.2.

In the frame of EURATOM (European Atomic Energy Community) PEBS (Long-term performance of Engineered Barrier Systems) project CIMNE (International Center for Numerical Methods in Engineering) a researcher group performed THO (Thermo-osmosis) and THM (Thermo-Hydro-Mechanical) analysis of the bentonite material which is used as a buffer. The buffer task of bentonite material used by the after the 15 years and 1000 years time periods, CODE_BRIGHT software has been

used to analyze the temperature changes caused by the heat energy produced by HLW wastes at various points in the bentonite material and in some points in the rock. At the end of 15 years and 1000 years time periods, the temperature changes resulting from the heat energy produced by HLW wastes were analyzed by CODE_BRIGHT software at various points in the bentonite material and at some points in the rock. The plan view of the analysed model is given in Figure 1.3.

Table 1.2 Research Issue on Long-term Safety in EBS (Engineering Barrier System) (Kim et al., 2011)

	Fuel	Canister	Buffer	Backfill
R (Radiological)	Radioactivity decay* Radiation attenuation/heat generation* Induced fission (criticality)*	Radiation attenuation/ heat generation*	Radiation attenuation/ heat generation*	Radiation attenuation/ heat generation*
T (Thermal)	Heat transport*	Heat transport*	Heat transport*	Heat transport*
H (Hydrological)	Water/gas transport*		Water transport unsatur.*** Water transport satur.* Gas transport/dissolution***	Water transport unsatur.* Water transport satur.*** Gas transport/dissolution*
M (Mechanical)		Deformation insert*** External deformation Cu** Inner deformation Cu**	Swelling* Mech. inter. buffer/backfill** Mech. inter. buffer/canister*** Mech. inter buffer/rock* Thermal expansion*	Swelling* Mech. inter. backfill/ rock***
	Thermal expansion/cladding failure*	Thermal expansion*		Thermal expansion*
C (Chemical)	Advection/diffusion* Resid. gas radiolysis/oxygen form.* Water radiolysis* Metal corrosion* Fuel dissolution*** Dissolution gap invent* Speciation radionuclides/ colloid formation** Helium production*	Corrosion insert*** Galvanic corrosion* SCC insert* Radiation effects* Copper corrosion*** SCC shell*** Grain growth copper*	Advection* Diffusion* Osmosis (salt effect)** Ion exch./sorption* Montmorillonite transf.*** Dissolution/prec. impurities* Colloid release/erosion*** Radiation-induced montmorillonite transf.* Radiolysis pore water* Microbial processes**	Advection* Diffusion* Osmosis (salt effect)** Ion exch./sorption* Montmorillonite transf.* Dissolution/prec. impurities** Colloid release/erosion** Radiation-induced transf.* Radiolysis pore water* Microbial processes**
Integration		HMC evolution damaged canister***	THM evolution unsaturated*** THMC evolution saturated***	
Radionuclide transport		RN transport near-field**	Advection** Diffusion** Sorption* Speciation* Colloid transport**	Advection** Diffusion* Sorption* Speciation*

*** : Major initiatives, ** : Moderate initiatives, * : Minor initiatives/monitoring during coming three-year period

As can be seen in Figure 1.3 in the plan view the distance between two shafts is 35.00 m from center to center, 2.00 m between two consecutive canisters in the same shaft and one canister length is 4.54 m. However, the perimeter of the canister is surrounded by bentonite material and there is rock material between two shafts.

It is known that many computer programs using finite element method can solve symmetrical models as axi-symmetrical. This approach shortens the solution time and allows more finite elements to be used, resulting in more precise solutions. In this context, the axi-symmetrical model of the system given in Figure 1.3 is given in Figure 1.4.

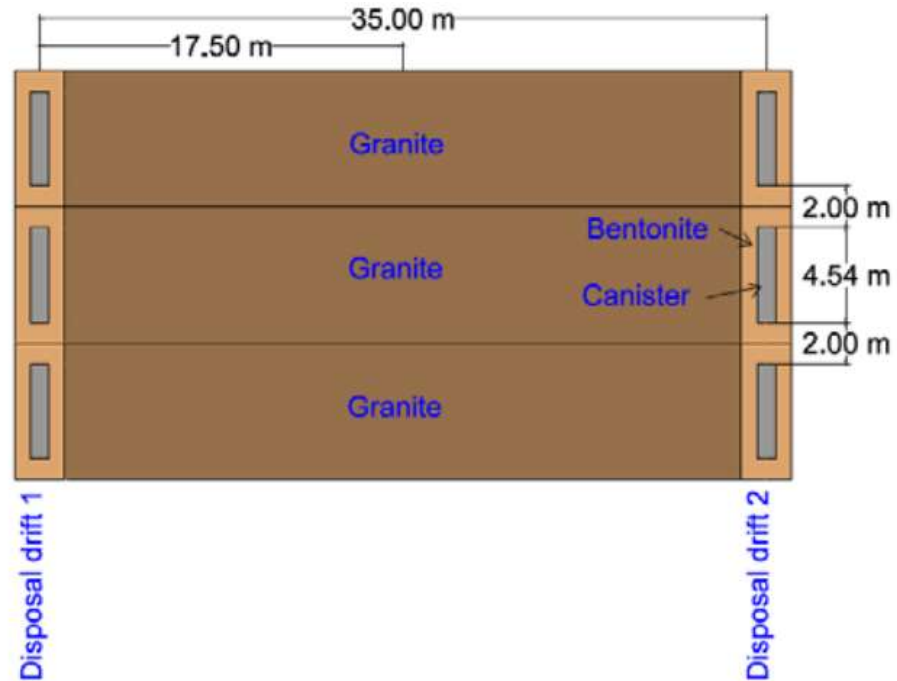


Figure 1.3 Top view of disposal drifts in the repository system (Wieczorek et al., 2014)

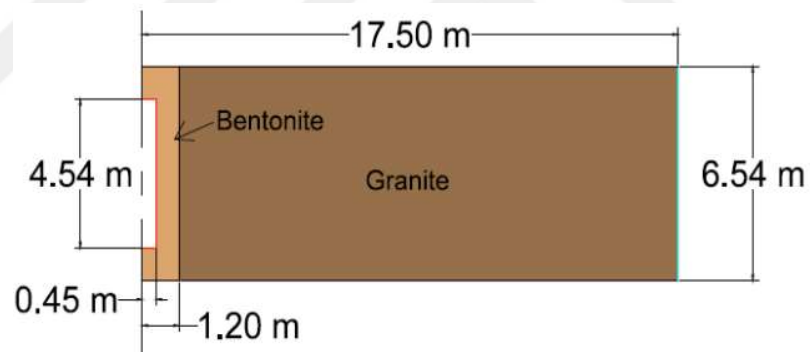


Figure 1.4 Size of the individual disposal cell (Wieczorek et al., 2014)

The two dimensional axi-symmetrical model which is given in Figure 1.4, was analyzed by CODE_BRIGHT program under 100 °C constant canister surface temperature and heat energy produced by spent fuel and spreading from the canister surface to the bentonite layer. These analyses were performed by CIMNE and the results for 1000 years are given in Figures 1.5 (a) and (b).

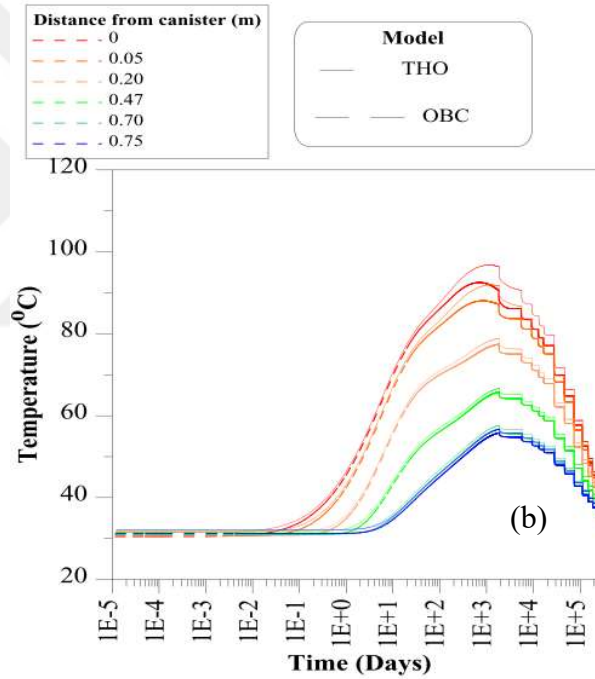
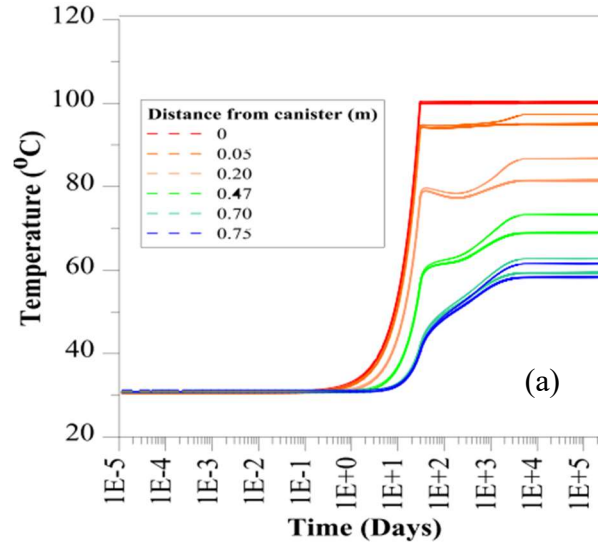


Figure 1.5 Evolution of temperature inside the bentonite buffer up to 365000 days (1000 years) at different positions from the canister: (a) Constant temperature at canister surface (b) Heat flux from canister surface (Wieczorek et al., 2014)

1.1.2 Thermal Conductivity of Soils

A rapid increase in the number of studies on the diversity of power structures has resulted in increased research into the thermal conductivity of soils. Heat transfer characteristics of soils vary with respect to some factors, such as water content, dry

density, pore water mineralogy and mineralogical composition (Ahn & Jung, 2017; Cai, Zhang, Puppala, & Liu, 2015; Fricke, Misra, Becker, & Stewart Jr, 2000; Omer, 2017; Tien, Chu, & Chuang, 2005). Therefore, it is necessary that the thermal conductivity of a soil subjected to different temperature gradients should be determined with respect to its characteristics specific to the environment.

The thermal conductivity coefficient is a measure that is usually indicated by “ λ ” in heat transfer equations and it shows the heat transfer capability of a material. The unit for the thermal conductivity coefficient is W/m-°C in the SI unit system, and W/m-K and W/m-°C units can be used interchangeably. The thermal conductivity coefficient is not a single measure to determine how much and how fast a substance can transmit heat. As can be seen in the general heat equation given in Equation (1.1), heat transfer capabilities of substances also depend on their heat capacities (c_p : J/kg-°C) and densities (ρ : kg/m³).

$$\frac{\partial}{\partial x} \left(\lambda_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda_z \frac{\partial T}{\partial z} \right) + \dot{q} = \rho c_p \frac{\partial T}{\partial t} \quad (1.1)$$

Equation (1.1) can be simplified to Equation (1.2) for a constant thermal conductivity coefficient (isotropic).

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{\dot{q}}{\lambda} = \frac{1}{\alpha} \frac{\partial T}{\partial t} \quad (1.2)$$

where “ α ” is the heat transfer coefficient (rate) expressed as $\lambda / (\rho c_p)$.

It is known that materials with high heat transfer coefficient values transmit heat faster than those with low heat transfer coefficient values. The term “ ρc_p ” in the denominator of “ α ” is called the heat capacity of a material. It means that a material with high heat capacity stores high amounts of energy and will require a greater amount of heat to increase its temperature. Similarly, it can be concluded that materials with low heat capacity values store less amounts of energy and will require a lower

amount of energy to increase their temperatures. In the literature, the definition of thermal resistivity is also indicated as the reverse of thermal conductivity value ($1/\lambda$). The unit of thermal resistivity is m-K/W and shown with an “R” symbol. Because materials with low thermal resistivity values have high thermal conductivity values, it is known that materials with low thermal resistivity transmit heat better compared to those with high thermal resistivity.

The thermal conductivity coefficient of composites can be obtained both theoretically and empirically. The thermal conductivity coefficient of mixtures is also used as the effective thermal conductivity coefficient and shown by a λ_f symbol in literature. Empirical equations found as a result of theoretical studies performed to calculate thermal conductivity coefficient of composites differ from each other in terms of material properties. Numerous models consider only thermal conductivity coefficients and volume fractions of composite components, while other models also consider grain shape, grain size structures, contact mode and contact factors. Serial, parallel and geometric models are the simplest models constructed to calculate the thermal conductivity values of two-component composites. These models are based on weighted arithmetic, harmonic and geometric average calculations and are given in Equations 1.3, 1.4 and 1.5, respectively. The term λ_f is the thermal conductivity coefficient of a composite, while λ_s (continuous phase) and λ_d (filling phase) are the thermal conductivity coefficients of composite constituents, respectively, and Θ is the volume fraction of the continuous phase of the composite.

$$\lambda_{f(serial)} = \left[\frac{\Theta}{\lambda_s} + \frac{1 - \Theta}{\lambda_d} \right]^{-1} \quad (1.3)$$

$$\lambda_{f(parallel)} = \Theta * \lambda_s + (1 - \Theta) * \lambda_d \quad (1.4)$$

$$\lambda_{f(geometric)} = \lambda_s^\Theta * \lambda_d^{(1-\Theta)} \quad (1.5)$$

Theoretical calculations based on an average calculation philosophy have turned into a detailed form over time. The Maxwell (1954) model is the primary one among these detailed calculations. This model accepts that the distributed phase does not

contact others and forms continuous transfer paths. The model mentioned above is given in Equation 1.6.

$$\lambda_{f(maxwell)} = \lambda_s \left[\frac{2\lambda_s + \lambda_d - 2(\lambda_s - \lambda_d) * \Theta}{2\lambda_s + \lambda_d + (\lambda_s - \lambda_d) * \Theta} \right] \quad (1.6)$$

The Maxwell model is a pioneering model in the published literature. That is why there are many modified Maxwell models. Maxwell–Hamilton, Maxwell–Eucken 1 and Maxwell–Eucken 2 equations are the most significant examples among these modified models. In addition to the Maxwell model, De Vries (1952), Johansen (1975), the Eucken (1932) and Kersten (1949) models are other important models constructed to calculate the thermal conductivity coefficients of composites. In addition to theoretical models constructed for calculating the thermal conductivity coefficient of composites, experimental studies have also developed considerably. Experimental methods are given in related ASTM (American Society for Testing and Materials standards). Table 1.3 shows some measurement methods, related standards and brief explanations.

Table 1.3 Thermal conductivity coefficient measurements and ASTM standard codes

METHODS	ASTM CODE	EXPLANATION
Guarded-Comparative-Longitudinal Heat Flow Technique	E1225-99	Thermal Conductivity of Solids by Means of the Guarded-Comparative-Longitudinal Heat Flow Technique
Hot Wire Method	C1113-99	Thermal Conductivity of Refractories by Hot Wire
Modulated Temperature Differential Scanning Calorimetry	E1952-01	Thermal Conductivity and Thermal Diffusivity by Modulated Temperature Differential Scanning Calorimetry
Hot Wire Method	D5334-00	Determination of Thermal Conductivity of Soil and Soft Rock by Thermal Needle Probe Procedure

The three most important factors affecting the thermal conductivity coefficient of soils are the dry density, water content and the percentage of fine particles. Thermal conductivity coefficient increases with increasing water content and dry density (Becker & Fricke, 1997). Becker and Ficker (1997) reported that when dry density increases in soils, particle contact will increase; thereby, increasing the thermal

conductivity coefficient. Similarly, for low water content, because there are voids between particles of a composite, the thermal conductivity coefficient will be less. Where water content is high, all particles will be surrounded by water film and a contact surface will form, which will increase the thermal conductivity coefficient. As shown in Figure 1.6, in stage 1, air voids are present between particles while they are filled with water in stages 2 and 3.

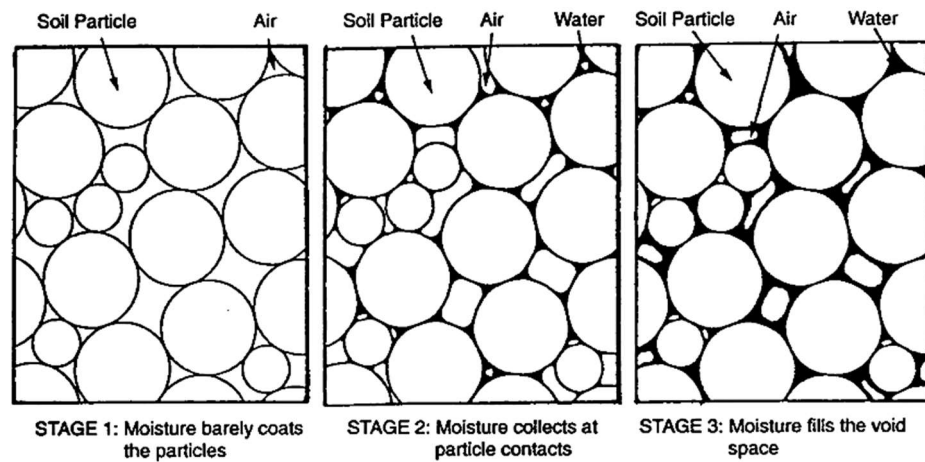


Figure 1.6 Saturation States of Granular Media (Becker & Ficker, 1997)

Because the thermal conductivity of water is much higher than that of air, the thermal conductivity coefficient increases with increasing water content in porous composites and coarse-grained materials.

Tien et al. (2005) revealed that the thermal conductivity of bentonite increased with increasing water content and dry density. In this study, it is seen from Figure 1.7 that when water content increases from 8% to 12%, the thermal conductivity value shows a sudden increase; when it is 16%, thermal conductivity reaches its peak value, and when it is further increased to 20%, the thermal conductivity trend is no longer upwards. It can be seen from Figure 1.8 that the thermal conductivity value of bentonite increases directly in proportion with dry density.

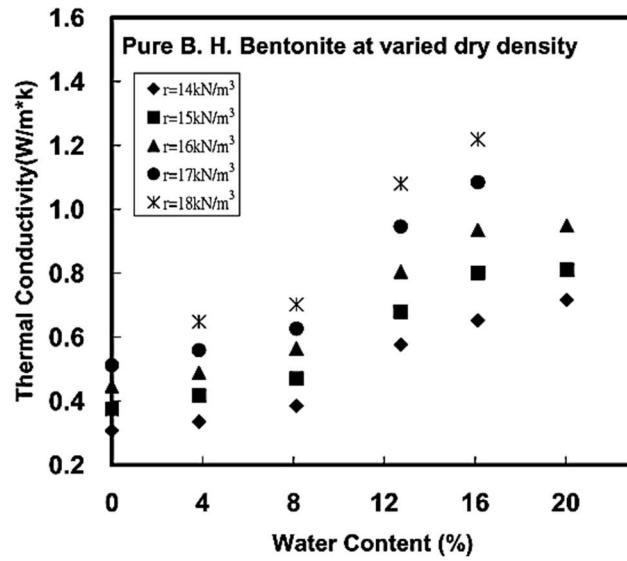


Figure 1.7 Thermal conductivity values of Bentonite with respect to water content (Tien et al., 2005)

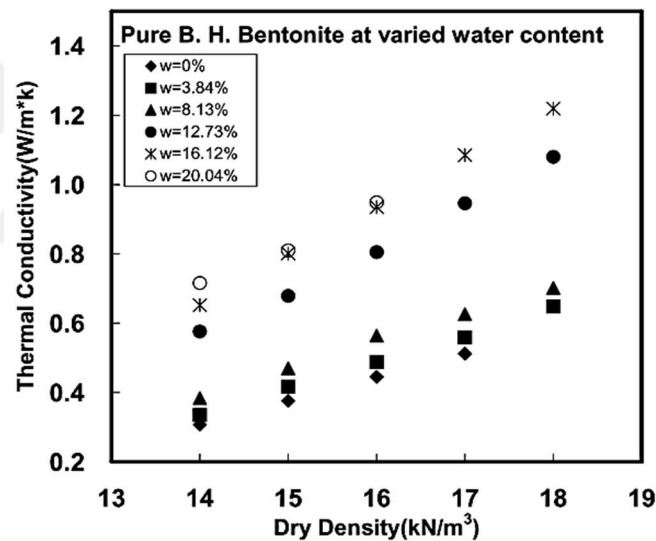


Figure 1.8 Thermal conductivity values of Bentonite with respect to dry density (Tien et al., 2005)

Cai et al. (2015) determined the thermal conductivities of clay, silt, fine sand and coarse sand samples – obtained from the Nanjing region in China – with respect to water content, grain diameter and dry density values. As indicated in Figure 1.9, according to the results obtained, when the water content and dry density values of silt samples increase, its thermal resistivity decreases, i.e. the thermal conductivity value increases. Thermal conductivity increased with increasing grain diameter of soils;

however, there was no linear relationship between grain diameter and thermal conductivity.

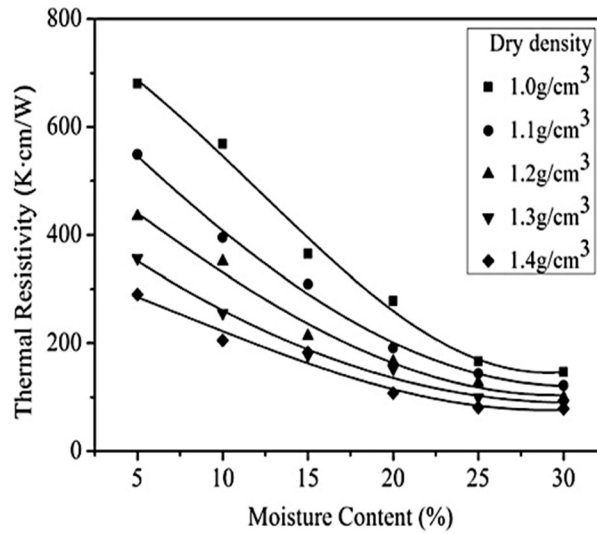


Figure 1.9 Relationship between thermal resistivity and moisture content of silt (Cai et al., 2015)

Ahn and Jung, (2017) revealed what amount of fine-grained materials changed the thermal conductivity coefficients of porous composite soil samples. It was also reported that fine-grained soils into coarse-grained soils and the results of the experiments showed that thermal conductivity of coarse-grained samples increased due to the increase in the amount of fine-grained materials. They also concluded that there was a direct proportional relationship between the density of coarse-grained materials and their thermal conductivity values. Another significant result obtained in that study is that the thermal conductivity value increased with decreasing porosity. When vertical loads were increased acting on samples from 10 kPa to 1000 kPa and thus decreased the void ratio in the sample; as a result, the thermal conductivity value increased, as shown in Figure 1.10.

Ahn and Jung (2017) provided two theoretical relationships for loose and dense cases, including the maximum fine grain size to fill coarse grains in sand mixtures. As can be seen in Figure 1.11, the void ratio is high in loose mixtures (Figure. 1.11 (a)) while it is low in dense mixtures (Figure 1.11 (b)).

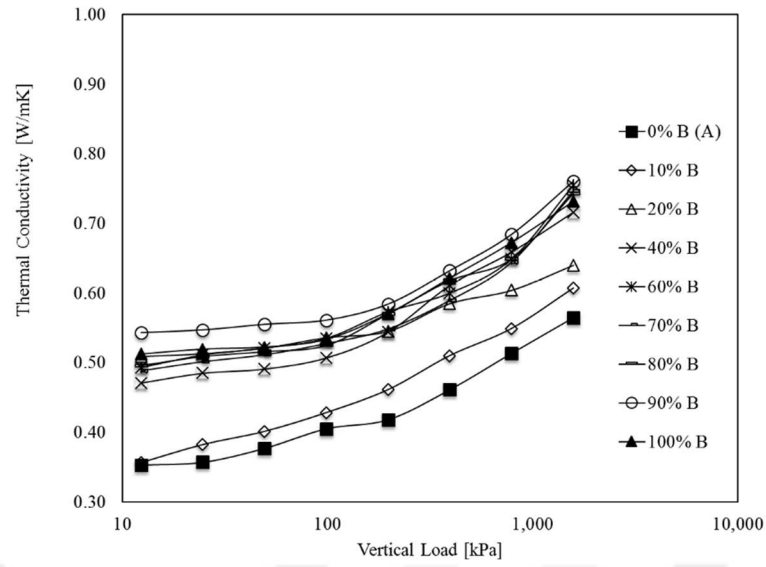


Figure 1.10 Vertical loads vs. thermal conductivity (Ahn & Jung, 2017)

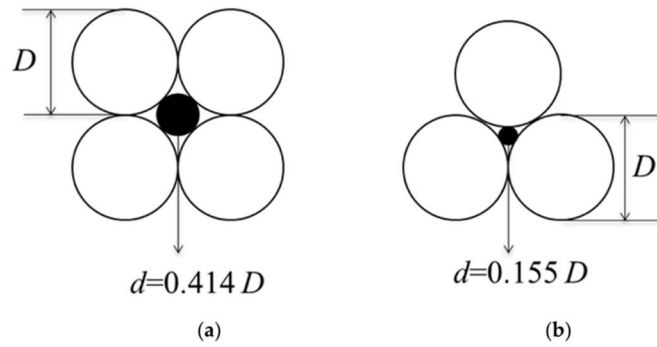


Figure 1.11 Theoretical pore body sizes of soil packing (“D” and “d” are diameters of the host and fine particles, respectively): (a) the loosest simple cubic packing and (b) the densest tetrahedral packing Ahn & Jung (2017)

The thermal conductivity coefficient of soils vary with respect to organic matter content (Figure 1.12), and thermal conductivity value decreases with increasing organic matter percentage (Omer, 2017). When organic matter content is increased from 5% to 30%, the thermal conductivity coefficient decreases from 0.3 W/m·K to 0.1 W/m·K level. Evaluating in terms of dry density, water content and void ratio values, it can be said that organic matter content has a considerable effect on the thermal conductivity value.

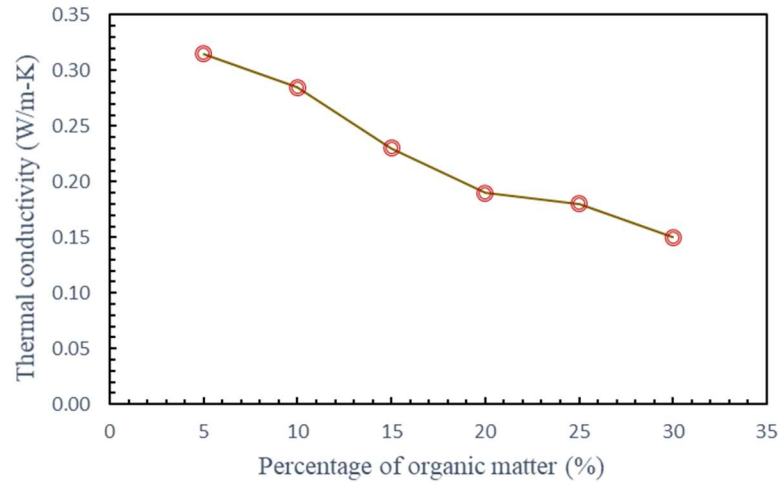


Figure 1.12 Soil thermal conductivity of clay loam as a function of organic matter (Omer, 2017)

It can be seen from the studies performed by Omer (2017) that the thermal conductivity coefficient decreased by 50% when the organic matter content increased.

1.1.3 Boron Minerals

Boron is a very important mineral for Turkey. Turkey's reserves are ranked first worldwide in terms of boron resources. Turkey has 63% of the world reserves. While the reserve life of Turkey's boron mines is 412 years, boron reserves in the U.S.A., which is the country with the second largest reserve in the world, has a 76 year life span. Considering the consumption growth rate of world reserves, it is highly possible that in 50 to 80 years from now Turkey's boron deposits will be the only boron resources remaining in the world (TMMOB-Maden Mühendisleri Odası, 2005)

Industrially important boron compounds include kernite, probertite, szaibelyite, datolite, sassolite, borax decahydrate, borax pentahydrate, anhydrous borax, boric acid, sodium perborate, anhydrous boric acid, and hydroboracite – under the main borax groups (tincal, sodium-based boron compounds), colemanite (calcium-based boron compounds) and ulexite (sodium-calcium-based boron compounds).

The value of boron minerals is usually measured in terms of B_2O_3 (boric oxide) content, and those with high amounts of the B_2O_3 compound are considered to be more

valuable (Yılmaz, 2002). Boron is an element that shows both metallic and nonmetallic properties. It is not present in nature in elemental form, but found as minerals in compounds called borates that include oxygen, carbon and other elements. The glass industry is responsible for 42% of boron use worldwide. Boron is included in glass in the form of boron compounds like boron oxide, anhydrous borax and boric acid or as some minerals like borax, or colemanite. It decreases expansion and thus increases thermal shock resistance. Boron significantly reduces thermal expansion of glass, protects it against acids and scratches, provides durability against vibration, high temperature and thermal shocks; thus, it is very important in manufacturing heat-resistant glass equipment, as well as high-quality glass to be used in electronic and space research. Boron compounds and boron fibers are used in plastics or metals for high durability and flexibility. In industry, boron combines high temperature resistance, flexibility and light weight with performance and manufacturing ease. Boron is one of 16 basic plant foods crucial for plant growth. It has been determined that compounds containing boric acid or boron are not genotoxic, carcinogenic, mutagenic, allergic or endocrine disruptors (Sahin, 2014). Boron has many areas of use in industry, but other areas will not be covered in this study.

Boron is indicated by the symbol B in the periodic table. Its atomic number is 5, its atomic weight is 10.81, and it is a semiconductor, showing both metallic and nonmetallic characteristics. It is the first element of the 3A group of the periodic table, being the lightest one. Its solid state electron configuration is $1s^2 2s^2 2p^1$. The element Boron has ^8B , ^{10}B , ^{11}B , ^{12}B and ^{13}B isotopes. Its most stable isotopes are ^{10}B and ^{11}B . The ^{10}B isotope shows a very high thermal neutron affinity characteristic. In other words, the boron nucleus captures neutrons emerging from nuclear waste areas to form more stable compounds, decreasing the existing radiation (Tombal, Özkan, Ünver, & Osmanlioğlu, 2016). Therefore, it can be used with nuclear materials and in nuclear power plants. Turkey has boron ore deposits with high amounts of the ^{10}B isotope. The various properties of boron compounds formed with metallic or nonmetallic elements mean that boron compounds are used in numerous industries. Boron compounds behave like nonmetallic compounds; however, pure boron conducts electricity like carbon.

Crystallized boron looks like diamond in terms of appearance and optical properties, and it can be almost as hard as diamond. Boron is the fifty-first most commonly found element in the earth's crust. Boron is never found in nature in a free state. It is known that there are approximately two hundred and thirty types of boron minerals in nature. One of the commonly occurring boron minerals is tourmaline, which is an alumino-borosilicate mineral, and it can include up to 10% boron. However, in industry, alkaline and earth-alkaline boron minerals, such as ulexite ($\text{NaCaB}_5\text{O}_9 \cdot 8\text{H}_2\text{O}$), colemanite ($\text{Ca}_2\text{B}_6\text{O}_{11} \cdot 5\text{H}_2\text{O}$), tincal ($\text{Na}_4\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$) and kernite ($\text{Na}_2\text{B}_4\text{O}_7 \cdot 4\text{H}_2\text{O}$) are used. Its commercial mineral ores are limited and Turkey and the U.S.A have the highest deposits. The chemical properties of elemental boron depend on its morphology and grain size. Amorphous boron of micron size easily – and sometimes intensively – reacts, while crystallized boron does not. Boron reacts with water at high temperatures forming boric acid and some by products. Its reaction with mineral acids can be slow or explosive depending on concentration and temperature, and the main product formed is boric acid. The physical properties of elemental boron are shown in Table 1.4.

Table 1.4 Physical properties of elemental boron

Boiling Point	4275 K - 4002°C - 7236°F
Thermal Expansion Coefficient	0.0000083 cm/cm/°C (0°C)
Thermal Conductivity	0.274 (W/m-K)
Heat of Vaporization	489.7 kJ/mol
Melting Point	2573 K - 2300°C - 4172°F
Specific Heat	1.02 J/g- K

1.2 Scope of This Study

Heat increases in soils may negatively affect engineering behavior. For example, increases in hydraulic conductivity values due to thermal effects in impermeable sand–bentonite barriers used for nuclear waste isolation will cause irreversible environmental pollution. For that reason, heat increase in the buffer and host rock should be controlled.

In this thesis, the thermal conductivity of boron added sand-bentonite mixtures determined. Instead of bentonite material used as a buffer around canister where waste is stored in nuclear waste repositories, boron added sand-bentonite mixtures were used in this thesis, single and double layer structures were designed separately and analyzed with the help of two different computer program using finite element method. In this study, the thermal conductivities of sand–bentonite mixtures with added boron were experimentally and numerically studied, and their uses in the heat isolation of structures that are in contact with soil and which transfer substantial heat to their surroundings were investigated.



CHAPTER TWO

MATERIAL CHARACTERIZATION AND METHODS

2.1 Material Characterization

In the first part of this study, the thermal conductivities of sand–bentonite mixtures were determined in the presence of ulexite, colemanite and tincal boron minerals. Bentonite was purchased from the Eczacıbaşı Esan Mining Co., while ulexite, colemanite and tincal were obtained from Eti Mining General Directorate. All materials were kept in the supplier's packaging to avoid any possibility of unwanted activity. The bentonite samples were oven dried (105°C), crushed and sieved through a 0.425 mm sieve (No.40). Grain size distribution, liquid limit, plastic limit and specific gravity values of soil samples were determined in accordance with ASTM D422 (1999a), ASTM D4318 (1999b) and ASTM D854 (1999c) standards.

Sand was sieved through a No.6 sieve, while ulexite, colemanite and tincal samples were sieved through a No.40 sieve. The physico-chemical properties of sand, bentonite and boron mineral samples are given in Tables 2.1 and 2.2, respectively.

Table 2.1 Properties of the sand and bentonite

	Sand	Bentonite
Specific gravity	2.65	2.697
Liquid limit (%)	---	468
Plastic limit (%)	---	53.7
Clay (%)	12	60

Table 2.2 Properties of the boron minerals

	Ulexite	Colemanite	Tincal
Specific Weight (g/cm ³)	1.96	2.42	1.73
Molecular Weight (g/mol)	405.21	411.08	381.37
Heat Capacity (J/g·°C)	25.10	15.40	4.00
Thermal Conductivity (W/m-K)	0.482	0.526	0.704
Specific Surface Area (m ² /g)	<1	3.30	13.55
Surface Tension (mN/m)	68.64	64.78	67.19

2.2 Methods

2.2.1 Sample Preparation

Sample preparation was performed in two main groups. In the first group of samples, the ratio of bentonite to the sum of bentonite and sand was 10%, while that ratio was 20% in the second group of samples. While preparing the two main sample groups, the sand–bentonite ratio was kept constant in relation to the total solid material. For example, when 5% boron was added to samples with 10% bentonite, the remaining 95% was composed of 10% bentonite and 90% sand. Thus, the material ratios of the sample were 5% boron, 9.5% bentonite and 85.5% sand. The purpose of this was to equalize the sand–bentonite attraction in the same-group samples and examine the effects of boron additives in different ratios in a more realistic way.

The mixtures were named in a such way that the boron percentage and the first letter of the mineral name came first, followed by the sand percentage with an S suffix, and lastly the bentonite percentage with a B suffix. To illustrate, 5U-85.5S-9.5B notation indicates that the sample has 5% ulexite, 85.5% sand and 9.5% bentonite. All samples prepared in this study are shown with their notations in Table 2.3.

Table 2.3 All samples used in experiments with their notations

Group	Additives	Ulexite	Colemanite	Tincal
10%Bentonite	5 %	5U-85.5S-9.5B	5C-85.5S-9.5B	5T-85.5S-9.5B
	10%	10U-81S-9B	10C-81S-9B	10T-81S-9B
	15%	15U-76.5S-8.5B	15C-76.5S-8.5B	15T-76.5S-8.5B
20%Bentonite	5%	5U-76S-19B	5C-76S-19B	5T-76S-19B
	10%	10U-72S-18B	10C-72S-18B	10T-72S-18B
	15%	15U-68S-17B	15C-68S-17B	15T-68S-17B

2.2.2 Thermal Conductivity Tests

As mentioned in the introduction, the thermal conductivities of porous composite soils with sand basically depend on the dry density, porosity, water content, fine-grained material content and organic matter content. Thus, to determine how boron

additives affect the thermal conductivity coefficients of sand–bentonite mixtures, the void ratio was kept constant at 0.74 in all samples. This value was taken as the void ratio of the 10% bentonite–90% sand mixture without any boron additives. The void ratio value used in calculations was found using Equations (2.1) to (2.8).

$$\delta_{dry} = \delta_n / (1 + \omega_{opt}) \Rightarrow \delta_n \quad (2.1)$$

$$\delta_n = W_{total} / V_{vessel} \Rightarrow W_{total} \quad (2.2)$$

$$W_{total} = W_{soil} + \omega_{opt} * W_{soil} \Rightarrow W_{soil} \quad (2.3)$$

$$W_{soil} = \delta_{soil} * V_{soil} \Rightarrow V_{soil} \quad (2.4)$$

$$V_{soil} = V_{total} - V_{void} \Rightarrow V_{void} \quad (2.5)$$

$$e = V_{void} / V_{total} \quad (2.6)$$

$$\delta_{dry,new} = (G_s * \delta_{water}) / (1 + e) \quad (2.7)$$

$$\delta_{n,new} = \delta_{dry,new} * (1 + \omega_{opt}) \quad (2.8)$$

In addition, all samples were prepared at their optimum water contents. The effects of void ratio and water content on thermal conductivity are important because the thermal conductivity coefficients of air and water are 0.024 and 0.607 W/m-K, i.e., they are very low. Optimum water content and maximum dry density values were determined with the help of the Standard Proctor Compaction Test (ASTM D-698, 2012) By using a pre-calculated specific weight (G_s) and optimum water content (ω_{opt}), values for the mixtures as well as a void ratio of 0.74 – by means of Equations (2.7) and (2.8) – the new dry density $\delta_{dry,new}$ ($\frac{g}{cm^3}$) and new wet density $\delta_{n,new}$ ($\frac{g}{cm^3}$) values were obtained. The values obtained are shown in Table 2.4. The boron, sand, distilled water and bentonite weight values used in samples were determined by using the $\delta_{n,new}$ values shown in Table 2.4. All calculated weight values are shown in Table 2.5.

Table 2.4 Optimum water content, specific weight, new dry and wet density values of samples

Group	Composite	ω_{opt}	G_s	$\delta_{dry,new}$	$\delta_{n,new}$
10% Bentonite	90S-10B	14.00%	2.636	1.722	1.963
	5U-85.5S-9.5B	15.90%	2.671	1.535	1.779
	10U-81S-9B	13.20%	2.688	1.545	1.749
	15U-76.5S-8.5B	13.00%	2.697	1.550	1.752
	5C-85.5S-9.5B	14.80%	2.597	1.493	1.713
	10C-81S-9B	12.90%	2.617	1.504	1.698
	15C-76.5S-8.5B	12.80%	2.621	1.506	1.699
	5T-85.5S-9.5B	16.20%	2.683	1.542	1.792
	10T-81S-9B	18.50%	2.697	1.550	1.837
	15T-76.5S-8.5B	19.00%	2.697	1.567	1.865
20% Bentonite	80S-20B	16.80%	2.579	1.482	1.731
	5U-76S-19B	16.80%	2.705	1.555	1.816
	10U-72S-18B	17.40%	2.711	1.558	1.829
	15U-68S-17B	15.30%	2.773	1.594	1.838
	5C-76S-19B	16.80%	2.625	1.509	1.762
	10C-72S-18B	16.40%	2.651	1.524	1.773
	15C-68S-17B	18.00%	2.704	1.554	1.834
	5T-76S-19B	16.90%	2.601	1.495	1.747
	10T-72S-18B	18.50%	2.685	1.543	1.829
	15T-68S-17B	20.50%	2.742	1.576	1.899

Table 2.5 The weight values of mixture contents

Group	Composite	Weight _{total} (g)	Weight _{soil} (g)	Weight _{water} (g)	Weight _{boron} (g)	Weight _{sand} (g)	Weight _{bentonite} (g)
10% Bentonite	90S-10B	1130.73	991.87	138.86	0.00	892.68	99.19
	5U-85.5S-9.5B	1024.78	884.19	140.59	44.21	755.99	84.00
	10U-81S-9B	1007.28	889.82	117.46	88.98	720.75	80.08
	15U-76.5S-8.5B	1008.86	892.80	116.06	133.92	682.99	75.89
	5C-85.5S-9.5B	986.93	859.70	127.24	42.98	735.04	81.67
	10C-81S-9B	978.07	866.32	111.75	86.63	701.72	77.97
	15C-76.5S-8.5B	978.70	867.64	111.06	130.15	663.75	73.75
	5T-85.5S-9.5B	1032.05	888.17	143.88	44.41	759.38	84.38
	10T-81S-9B	1057.97	892.80	165.17	89.28	723.17	80.35
	15T-76.5S-8.5B	1074.25	902.73	171.52	135.41	690.59	76.73
20% Bentonite	80S-20B	997.17	853.74	143.43	0.00	682.99	170.75
	5U-76S-19B	1045.88	895.45	150.44	44.77	680.54	170.14
	10U-72S-18B	1053.59	897.43	156.15	89.74	646.15	161.54
	15U-68S-17B	1058.41	917.96	140.45	137.69	624.21	156.05
	5C-76S-19B	1014.95	868.97	145.99	43.45	660.41	165.10
	10C-72S-18B	1021.49	877.57	143.92	87.76	631.85	157.96
	15C-68S-17B	1056.24	895.12	161.12	134.27	608.68	152.17
	5T-76S-19B	1006.53	861.02	145.51	43.05	654.38	163.59
	10T-72S-18B	1053.26	888.83	164.43	88.88	639.96	159.99
	15T-68S-17B	1093.77	907.70	186.08	136.15	617.23	154.31

For the samples used in thermal conductivity measurements, square section containers of $12\text{ cm} \times 12\text{ cm} \times 4\text{ cm}$ were made from a special wooden material, whose water absorption capacity is very low (Figure 2.1). Samples were laid down in containers using a trial and error method with a certain numbers of compaction effort to produce four layers, and then compacted with a wooden tamper.



Figure 2.1 Custom-engineered sample container (Personal archive, 2018)

Before compaction, the dry materials were first adequately mixed in dry and clean plastic cups; the water contents given in Table 2.5 were gradually added into the solid materials and mixed homogeneously with a spatula. The completely homogenized mixtures were put in air-vacuum cups and kept for 24 hours. After that, the samples were removed from the cups and mixed again for five minutes.

After completing the mixing, compaction was applied. The energy used for compaction was provided by hand, and after compaction, the materials with pre-calculated amounts were squeezed into the sample containers. It was assumed that the void ratios of all samples after compaction would be theoretically around 0.74. Compaction was started from position “a”, as shown in Figure 2.2 and region 1 was compacted. After that, the sample container was rotated in “a” counterclockwise direction by 90° around its lower left edge to obtain position “b” and then region 4 was compacted. The same operation was repeated for positions “c” and “d”. The aim was to provide the same energy for each region during compaction and make the upper surfaces of samples horizontal after compaction because faulty measurements are obtained on non-horizontal surfaces.

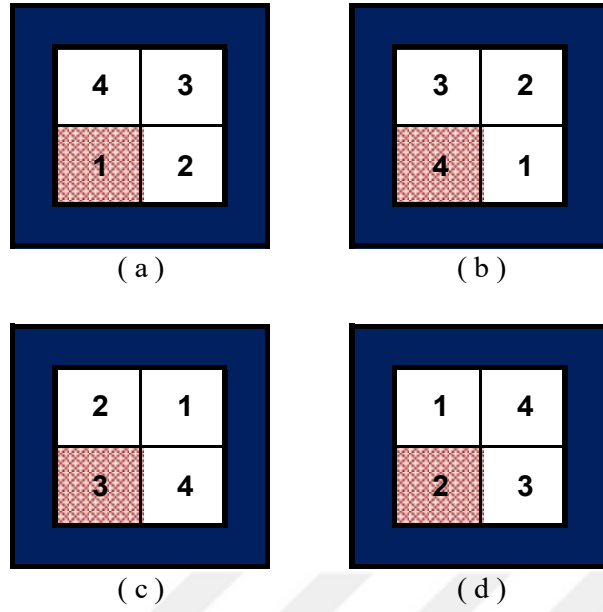


Figure 2.2 Compaction order for each layer

After completing the compaction, samples were packaged in such a way that air could not pass inside in vacuum containers, and thermal conductivity measurements were then started. Thermal conductivity measurements were performed by Shotherm QTM-D2 equipment (Figure 2.3) running the Hot-Wire method. The equipment was made available in the Energy Laboratory of the Department of Mechanical Engineering of Dokuz Eylül University.



Figure 2.3 Shotherm QTM-D2 measuring device (Personal archive, 2018)

All measurements were done at room temperature and the formation of temperature differences in the samples was prevented. Before starting measurements, equipment

calibration was performed by measuring a sample with a thermal conductivity value of 0.241 W/m-K. Measurement was performed by placing the Shotherm QTM-D2 equipment (Figure 2.3) horizontally on the sample and leaving it for 60 seconds. The experimental equipment calculates measurement results using Equation (2.9) and provides the results on its hardwired screen in W/m-K units to a sensitivity of three decimal places.

$$\lambda = F * \frac{Q \ln(t_1/t_2)}{T_2 - T_1} - H \quad (2.9)$$

where F and H are constants specific to the device, Q is the amount of heat flux provided to the heater wire, t_1 and t_2 are measurement times, and T_1 and T_2 are temperature values measured at t_1 and t_2 times, respectively. Measurements were done over five different zones of each sample and measurement photos are given in Figure 2.4.

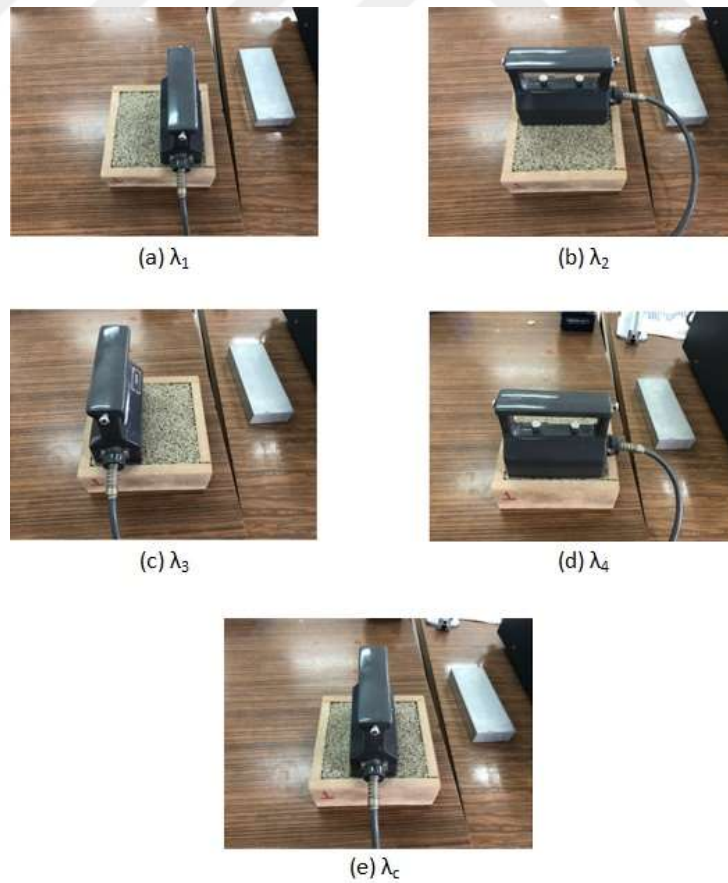


Figure 2.4 Measurement of thermal conductivity over five different zones (Personal archive, 2018)

As given in Figure 2.4, as a result of measurements obtained from five different zones of the samples, the homogeneous nature of the composite was studied, and its thermal conductivity coefficient was measured more precisely. As will be discussed in the results section, these five different measurement results were analyzed in terms of significance, and it was determined after a statistical approach, which value – or average of which values – would be used.

2.3 Finite Element Model for Thermal Analysis of Buffer Rounded Hlw Canister

The function and importance of bentonite during disposal of nuclear HLW was described in the introduction section. This chapter explains and details the finite element model used to investigate the use of boron-added sand–bentonite mixtures around the canister as a buffer in terms of its thermal aspects. Figure 2.5 (a) and (b) shows the plan geometry of the analysis area.

The construction of this geometry was inspired by the study of Wieczorek et al., (2014). As seen in Figure 2.5 (a) and (b), the distance between two shafts is 35.0 m from center to center. The distance between two successive canisters in the same shaft is 2.0 m. The length of the canister with buffer is 6.54 m. Wieczorek et al., (2014) designed the buffer as single layer using only bentonite. In the model constructed for this study, the system was modeled with a single layer and double layer buffer, similar to the model constructed by Wieczorek et al., (2014) and the results obtained are given in Chapter 4. The objectives of using boron-added sand–bentonite mixtures rather than pure bentonite for the buffer design are as follows:

1. Sand added to the mixture enhances strength properties.
2. Bentonite was used due to its high-swelling potential and hydraulic conductivity values.
3. Colemanite was used due to its neutron capture characteristics, i.e. for use as a radioactive barrier.
4. A sample with added tincal was used to decrease the temperature of the layer including colemanite.

5. Boron was used to increase the strength of the material under high thermal stresses to function as a buffer.

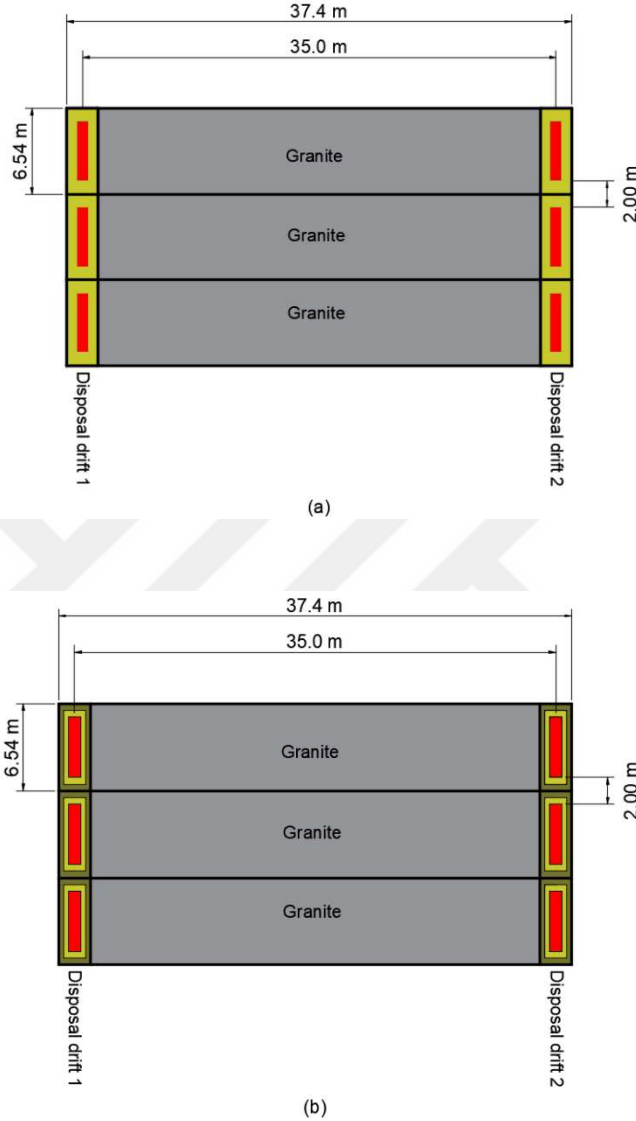


Figure 2.5 The plan geometry of the disposal drifts in the repository system (adapted from Wiczorek et al., 2014): (a) Single-layer buffer, (b) Double-layer buffer

The canister and materials used as buffer material in the analysis are shown in Figure 2.6 (a) and (b). As shown in Figure 2.6, the barrier was designed as a single and a double layer. For boron-added sand–bentonite mixtures, 15C-68S-17B material was assigned to the first layer while 15T-68S-17B material was the second layer. The reason for this is that the thermal conductivity (λ_f) value of 15T-68S-17B is higher than that of 15C-68S-17B. Another reason for using the samples with colemanite as

the first layer is due to the high neutron capture capability of colemanite (Tombal et al., 2016).

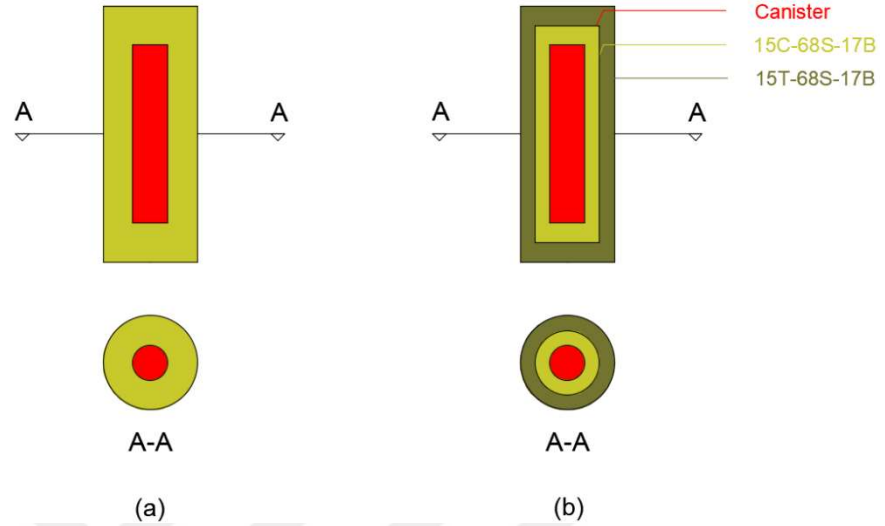


Figure 2.6 An A-A cross sectional view of the canister and material types with: (a) Single-layer buffer, (b) Double-layer buffer

The intended uses of colemanite material in nuclear power plants were explained in the introduction section. Colemanite-added sand–bentonite mixtures that function as a barrier in HLW isolation should be considered in terms of achieving thermal and hydraulic conductivity criteria and also preventing radiation leakage to the surroundings by capturing radioactive neutron particles released from spent fuel. Figure 2.7 (a) and (b) shows a canister and its single and double-layer buffer geometry.

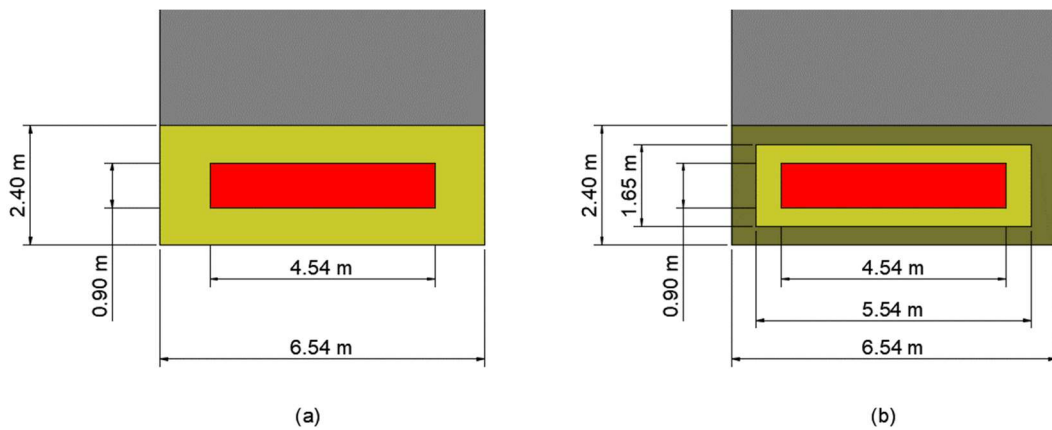


Figure 2.7 The geometry of Individual disposal cell: (a) Single layer buffer, (b) Double layer buffer

As can be seen in Figure 2.7 (a), the length and diameter of the canister is 4.54 m and 0.90 m, respectively. In the single layer system, buffer thickness is 0.75 m on the body while 1.00 m on the bottom. In the double layer system (Figure 2.7 (b)), the first and second buffer thicknesses are equal (3.75 m) on the body and equal on the bottom of canister (0.50 m). The $\frac{1}{2}$ model used in the analysis is shown in Figure 2.8 (a) and (b). The reason for using the $\frac{1}{2}$ model is because it is axi-symmetrical around the y axis.

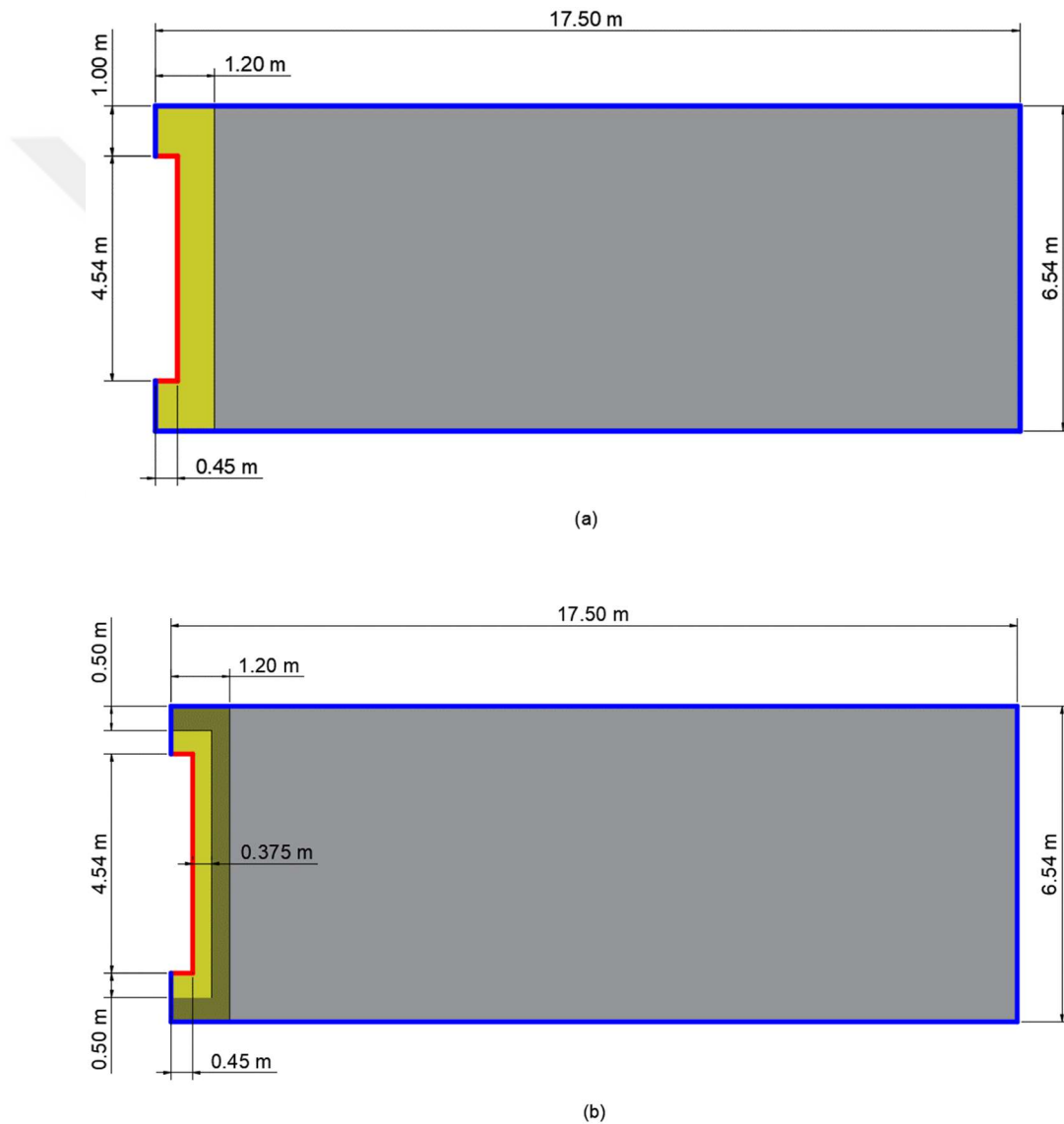


Figure 2.8 The axi-symmetrical model used in the FEM analysis: (a) Single-layer buffer (Wieczorek et al., 2014), (b) Double-layer buffer

CHAPTER THREE

RESULTS OF THE TESTS AND ANALYSES

3.1 Thermal Conductivity Results

Thermal conductivity measurements were performed over five different zones of all the samples using the Shotherm QTM-D2 equipment and the results are given in Tables 3.1 to 3.6. The values of λ_1 , λ_2 , λ_3 , λ_4 , and λ_c given in the tables indicate the measurement results at the (a), (b), (c), (d) and (e) zones shown in Figure 2.4.

Table 3.1 Thermal conductivity measurements of 10% bentonite mixtures with added ulexite

10% Bentonite			
Ulexite	5%	10%	15%
λ_1	0.870	1.095	1.084
λ_2	0.817	1.189	1.431
λ_3	0.882	1.021	1.230
λ_4	1.359	1.014	1.103
λ_c	1.167	1.110	1.216

Table 3.2 Thermal conductivity measurements of 10% bentonite mixtures with added colemanite

10% Bentonite			
Colemanite	5%	10%	15%
λ_1	0.777	0.937	1.073
λ_2	0.905	0.901	0.875
λ_3	0.947	1.071	1.167
λ_4	0.765	0.916	1.044
λ_c	1.138	1.146	1.125

Table 3.3 Thermal conductivity measurements of 10% bentonite mixtures with added tincal

10% Bentonite			
Tincal	5%	10%	15%
λ_1	1.110	1.245	1.408
λ_2	1.110	1.256	1.426
λ_3	1.118	1.298	1.394
λ_4	1.377	1.201	1.439
λ_c	0.877	1.198	1.547

Table 3.4 Thermal conductivity measurements of 20% bentonite mixtures with added ulexite

20% Bentonite			
Ulexite	5%	10%	15%
λ_1	0.924	1.264	1.419
λ_2	0.986	1.319	1.395
λ_3	1.080	1.297	1.449
λ_4	0.911	1.301	1.427
λ_c	0.972	1.273	1.403

Table 3.5 Thermal conductivity measurements of 20% bentonite mixtures with added colemanite

20% Bentonite			
Colemanite	5%	10%	15%
λ_1	1.254	1.357	1.427
λ_2	1.327	1.396	1.431
λ_3	1.264	1.356	1.414
λ_4	1.297	1.367	1.404
λ_c	1.246	1.339	1.398

Table 3.6 Thermal conductivity measurements of 20% bentonite mixtures with added tincal

20% Bentonite			
Tincal	5%	10%	15%
λ_1	0.785	0.998	1.688
λ_2	0.834	1.105	1.485
λ_3	0.958	1.112	1.465
λ_4	0.743	1.124	1.568
λ_c	0.898	1.021	1.439

To determine which values – or average of which values – shown in Tables 3.1 to 3.6 would be used, statistical analysis was carried out. A modified Thomson Tau technique was used to determine which measurement value was not significant compared to the other values. To examine the analysis more conveniently and simply, first all values were ranked and then the average value ($\bar{x}$) and standard deviation value (S) of the ranked values were calculated. After that, for each measurement data, the value of Ψ_i is calculated by using Equation (3.1) below:

$$\Psi_i = |x_i - \bar{x}| \quad (3.1)$$

After calculating the values of Ψ_i , the Modified Thomson Tau number (τ) is found from tables, depending on the data value. Lastly, the result obtained by multiplying the tau value by the standard deviation value is compared with the Ψ_i values and measurement data, where $\Psi_i > \tau \cdot S$ is considered to be insignificant. In such a case, the measurement is taken again or the average of the remaining data is obtained, and this value is used as the final value. Within this study, because 5 measurements were taken for each sample, the tau value was taken as 1.5712, two Thomson Tau test results are shown in Table 3.7 and 3.8. The red values should be considered insignificant.

Table 3.7 Statistical analysis of 5U-85.5S-9.5B measurement by the Thomson Tau method

Zone	Measurement	Ψ_i	$\bar{x}$	1.019
λ_4	0.817	0.202	S	0.234
λ_2	0.870	0.149	τ	1.5712
λ_1	0.882	0.137	$\tau \cdot S$	0.368
λ_c	1.167	0.148	λ_f	1.019
λ_3	1.359	0.340		

Table 3.8 Statistical analysis of 15C-76.5S-8.5B measurement by the Thomson Tau method

Zone	Measurement	Ψ_i	$\bar{x}$	1.057
λ_2	0.875	0.182	S	0.112
λ_4	1.044	0.013	τ	1.5712
λ_1	1.073	0.016	$\tau \cdot S$	0.176
λ_c	1.125	0.068	λ_f	1.102
λ_3	1.167	0.110		

Final thermal conductivity values for all samples to be used in calculations as a result of statistical analyses are shown in Table 3.9. As seen from the results in Table 3.9, the reference value in the 10% bentonite group was found to be 1.450 W/m-K, while it was 1.048 W/m-K in the 20% bentonite group. In other words, when considering the additive-free samples, the thermal conductivity value decreases with increasing bentonite percentage in sand-bentonite mixtures. Measurement results indicate that the lowest thermal conductivity coefficient (0.844 W/m-K) was found in the 5T-76S-19B sample while the highest value (1.489 W/m-K) was measured in 15T-68S-17B sample. In the group containing 10% bentonite, the lowest thermal

conductivity value (0.906 W/m-K) was observed in the sample with 5% colemanite. This result revealed that the thermal conductivity value could be decreased by 37.5% by adding only 5% colemanite into the sand–bentonite mixtures containing 10% bentonite. On the other hand, the thermal conductivity value increased proportionally when the amount of boron additive was increased from 5% to 15%. In the 20% bentonite group, the lowest value (0.844 W/m-K) was measured in the sample with 5% tincal. This result showed that the thermal conductivity coefficient could be decreased by 19.5% with the addition of 5% tincal in the sample group containing 20% bentonite. Considering all samples, it was seen that the thermal conductivity values of sand–bentonite mixtures could be decreased by 42% with appropriate boron additives.

Table 3.9 Thermal conductivity values of sand–bentonite mixtures with added boron

Group	Composite	λ_f (W/m-K)
10% Bentonite	90S-10B	1.450
	5U-85.5S-9.5B	1.019
	10U-81S-9B	1.086
	15U-76.5S-8.5B	1.158
	5C-85.5S-9.5B	0.906
	10C-81S-9B	0.994
	15C-76.5S-8.5B	1.102
	5T-85.5S-9.5B	1.118
	10T-81S-9B	1.240
	15T-76.5S-8.5B	1.417
20% Bentonite	80S-20B	1.048
	5U-76S-19B	0.948
	10U-72S-18B	1.291
	15U-68S-17B	1.419
	5C-76S-19B	1.278
	10C-72S-18B	1.355
	15C-68S-17B	1.415
	5T-76S-19B	0.844
	10T-72S-18B	1.041
	15T-68S-17B	1.489

Considering the effects of ulexite additives on the thermal conductivity values of sand–bentonite mixtures, when 5%, 10% and 15% ulexite additives were added into the 90S-10B mixture, the thermal conductivity values were 1.019, 1.086 and 1.158 W/m-K, respectively. In comparison, these values were measured to be 0.906, 0.994

and 1.102 W/m-K in the samples containing colemanite, while they were 1.118, 1.240 and 1.417 W/m-K in the samples with tincal. When 5%, 10% and 15% ulexite additives were added into the 80S-20B mixture, the thermal conductivity values were found to be 0.948, 1.291 and 1.419 W/m-K, respectively. In comparison, these values were measured to be 1.278, 1.355 and 1.415 W/m-K in the samples with colemanite, and 0.844, 1.041 and 1.489 W/m-K in the samples with tincal.

In the 90S-10B and 80S-20B mixtures, when the amount of ulexite additive increased, decreases were noted in the thermal conductivity values of 90S-10B mixtures, while the values for the 80S-20B mixtures first decreased and later increased compared to the additive-free sample. On the other hand, when the amount of colemanite additive increased, the thermal conductivity values for 90S-10B mixtures decreased while increases were observed in 80S-20B mixtures, which were higher than that of the additive-free sample.

Examining the effect of tincal in both main groups, the tincal additive decreased the thermal conductivity values in the 90S-10B mixtures, while it first decreased the thermal conductivity values in the 80S-20B mixtures, but a thermal conductivity value higher than that of the additive-free sample was obtained with the addition of 15% tincal.

Evaluating the 5% boron additives in general, the boron mineral that decreases the conductivity value most in the 10% bentonite group was colemanite, while it was tincal in the 20% bentonite group that increased the conductivity most. On the other hand, evaluating the conductivity values in terms of 15% boron additives, the mineral decreasing thermal conductivity most in the 10% bentonite group was colemanite, while tincal increased the thermal conductivity the most in the 20% bentonite group.

3.1.1 Calculation of Specific Heat, Heat Diffusion Coefficient and Volumetric Heat Capacity of Samples

In previous subsection, statistical analyses of measured data were made, and the final thermal conductivity results were presented. In this chapter, the specific heat, heat diffusion coefficient and volumetric heat capacity of each sample was calculated, and the effects of parameters on the heat transfer mechanism were investigated.

The heat capacity of a mixture ($c_{p,f}$) can be calculated with rule of mixtures theory (Thermtest, 2019) if the heat capacity of each material is known. Final heat capacity values of mixtures were calculated by using Equation (3.2):

$$c_{p,f} = \sum_{i=1}^n \frac{m_i}{m_t} * c_{p,i} \quad (3.2)$$

where m_i is the weight of material i in the mixture, m_t is total weight of the mixture, $c_{p,i}$ is the heat capacity of material i in the mixture and n is the number of materials in the mixture.

With the help of the calculated heat capacity values of the mixtures, the heat diffusion coefficient, α , and volumetric heat capacity, $\rho c_{p,f}$, values were calculated for each sample and presented in Table 3.10. In the calculations, the heat capacity values for water and bentonite were 4160 J/kg-K and 1000 J/kg-K, respectively. Heat capacity values for ulexite, colemanite and tincal were obtained from Table 1.4.

From Table 3.10 it is seen that the 90S-10B sample stores minimum heat energy and diffuse heat the fastest, while the 15U-68S-17B mixture stores maximum heat energy and diffuse heat the slowest. As stated in the introduction section, the heat transfer mechanism is mainly dependent on the thermal conductivity coefficient; on the other hand, it also related to the heat diffusion coefficient, i.e. specific heat and volumetric heat capacity. In this regard, the effects of the thermal characteristics of boron-added sand-bentonite mixtures on heat transfer were analyzed using

Code_Bright software. The analyses performed at this step were made to clarify only the material selection. The model analyzed is shown in Figure 3.1 (CODE_BRIGHT Tutorial-Thermal problem, 2019).

Table 3.10 Specific heat, heat diffusion coefficient and heat storage values of samples

Group	Composite	ρ	λ_f	$c_{p,f}$	α	$\rho c_{p,f}$
		kg/m ³	W/m-K	J/kg-K	m ² /s	J/m ³ -K
10% Bentonite	90S-10B	1963	1.450	1256	5.88E-07	2.47E+06
	5U-85.5S-9.5B	1779	1.019	2351	2.44E-07	4.18E+06
	10U-81S-9B	1749	1.086	3378	1.84E-07	5.91E+06
	15U-76.5S-8.5B	1752	1.158	4450	1.49E-07	7.79E+06
	5C-85.5S-9.5B	1713	0.906	1911	2.77E-07	3.27E+06
	10C-81S-9B	1698	0.994	2517	2.33E-07	4.27E+06
	15C-76.5S-8.5B	1699	1.102	3161	2.05E-07	5.37E+06
	5T-85.5S-9.5B	1792	1.118	1447	4.31E-07	2.59E+06
	10T-81S-9B	1837	1.240	1633	4.13E-07	3.00E+06
	15T-76.5S-8.5B	1865	1.417	1777	4.28E-07	3.31E+06
20% Bentonite	80S-20B	1731	1.048	1341	4.51E-07	2.32E+06
	5U-76S-19B	1816	0.948	2379	2.19E-07	4.32E+06
	10U-72S-18B	1829	1.291	3420	2.06E-07	6.26E+06
	15U-68S-17B	1838	1.419	4457	1.73E-07	8.19E+06
	5C-76S-19B	1762	1.278	1963	3.69E-07	3.46E+06
	10C-72S-18B	1773	1.355	2580	2.96E-07	4.58E+06
	15C-68S-17B	1834	1.415	3218	2.40E-07	5.90E+06
	5T-76S-19B	1747	0.844	1478	3.27E-07	2.58E+06
	10T-72S-18B	1829	1.041	1646	3.46E-07	3.01E+06
	15T-68S-17B	1899	1.489	1819	4.31E-07	3.45E+06

Figure 3.1 models the heat flow problem caused by nuclear waste storage across a rock mass. In the model constructed using the finite element method, the properties of the rock material did not change, and 4 models were used from a boron-added sand–bentonite mixture – rather than bentonite alone – and the temperature increase on the canister surface was investigated. Among the four samples used in this modeling, two of them (15T-76.5S-8.5B and 15T-68S-17B) had the same heat diffusion coefficient but different thermal conductivity coefficient values; the other two samples (80S-20B and 10T-72S-18B) had almost the same thermal conductivity coefficient but different heat diffusion coefficients. Table 3.11 shows properties of the four material types used in the analysis, and the thermal properties of the bentonite and rock materials used in the CODE_BRIGHT Tutorial-Thermal problem (2019).

Two different boundary conditions (BCs) were used in the simulation. The first one is the initial temperatures of the material surfaces. Initial temperatures of the bentonite and rock surfaces were 20°C and 25°C, respectively. The second boundary conditions are the flux BCs that include two different conditions. The first flux BC is to keep the temperature of the exterior boundaries of the model constant at 25°C, while the second one is the heat energy generation of 200 J/s diffusing from the canister surface to the buffer layer. The plan indicating the flow associated with the BCs is shown in Figure 3.2.

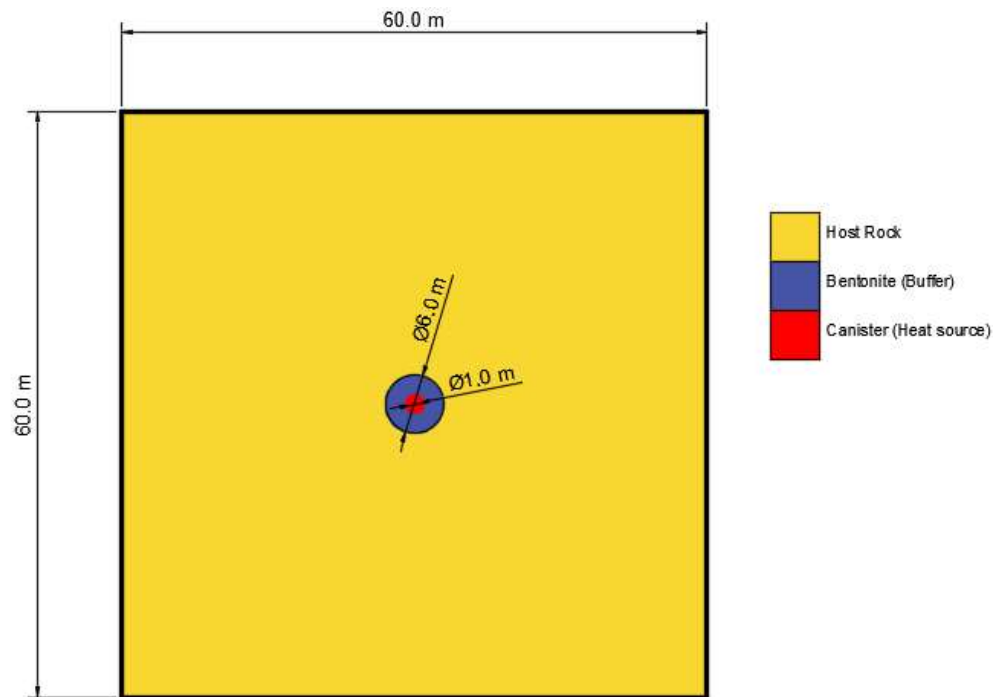


Figure 3.1 Geometry of the problem considered (CODE_BRIGHT Tutorial, thermal problem, 2019)

Table 3.11 Thermal properties of materials used in the model given in Figure 3.1

	kg/m ³	W/m-K	J/kg-K	m ² /s	J/m ³ -K
Material	ρ	λ_f	$c_{p,f}$	α	$\rho \cdot c_{p,f}$
15T-76.5S-8.5B	1865	1.417	1777	4.3E-07	3.31E+06
15T-68S-17B	1899	1.489	1819	4.3E-07	3.45E+06
80S-20B	1731	1.048	1341	4.5E-07	2.32E+06
10T-72S-18B	1829	1.041	1646	3.5E-07	3.01E+06
Bentonite (Tutorial)	2000	1.500	1000	7.5E-07	2.00E+06
Host Rock (Tutorial)	2500	3.000	800	1.5E-06	2.00E+06

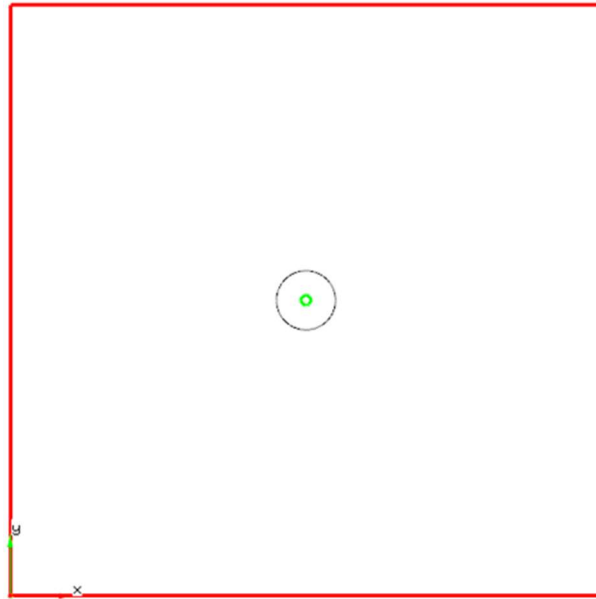


Figure 3.2 Flux boundary conditions

The red line in Figure 3.2 indicates flow associated with the BC at 25°C, while the green line indicates the heat energy of 200 J/s generated by the nuclear waste that diffuses over the canister surface. The mesh conditions used in the CODE_BRIGHT Tutorial-Thermal problem (2019) were used without change and the mesh results for the model are shown in Figure 3.3.

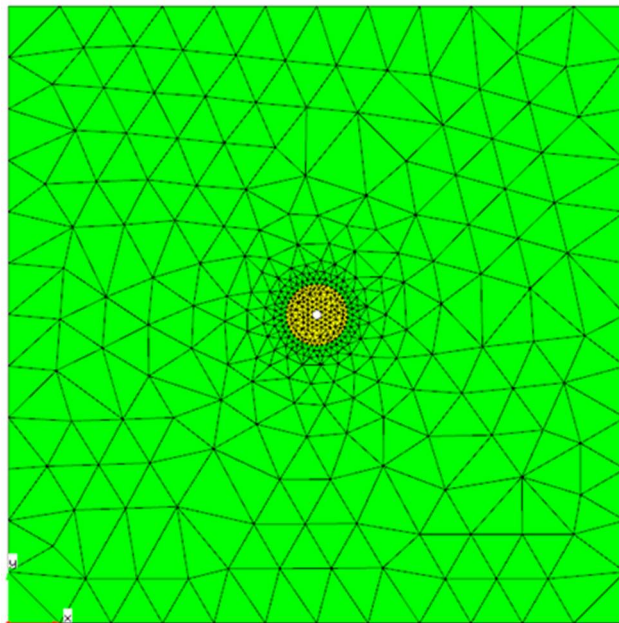


Figure 3.3 The finite element mesh of the model

To determine the accuracy of all inputs, the model given in the CODE_BRIGHT Tutorial-Thermal problem (2019) was simulated without changing the material properties, geometry, BCs and loading time (100 years) and the outcome of the analysis is shown in Figure 3.4.

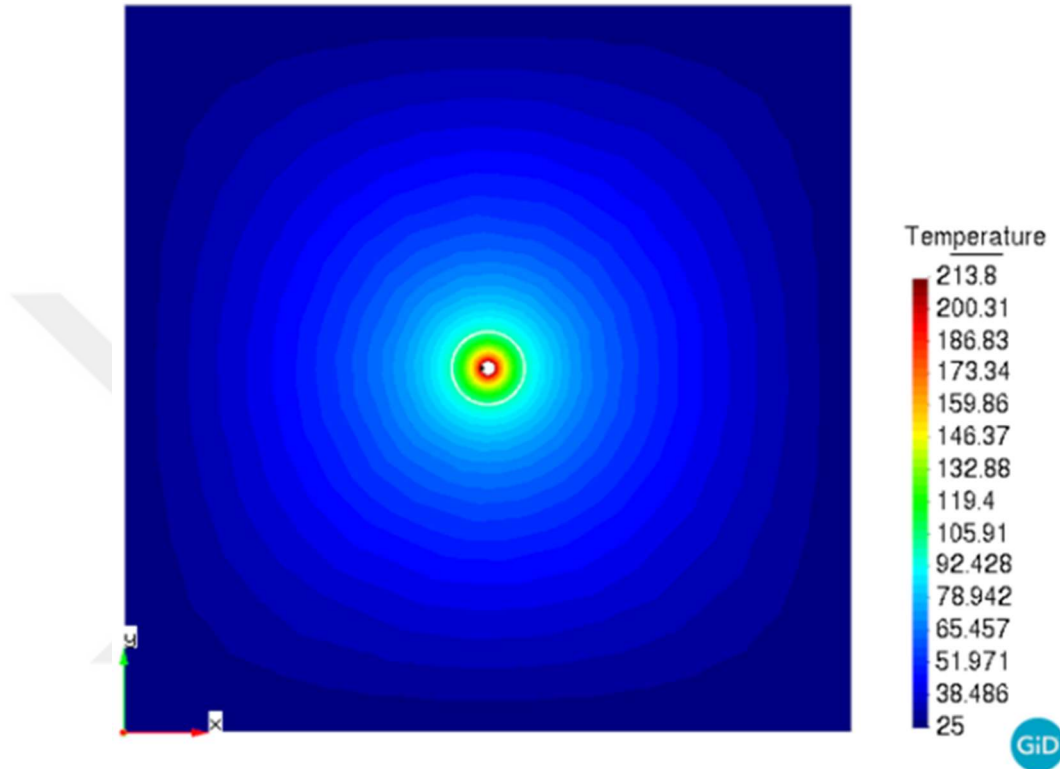


Figure 3.4 Analysis result of thermal problem in CODE_BRIGHT Tutorial (2019) by using GiD

The results given in Figure 3.4 exactly coincide with Figure 3.53 given in CODE_BRIGHT Tutorial-Thermal problem (2019) chapter. From this point of view, in this study, the thermal parameters of bentonite were exchanged with those of the four samples selected from boron-added sand-bentonite mixtures, and temperature–time graphs of the point on the canister surface with coordinates [29.5;30.0], and the point in the host rock with coordinates [26.0;30.0] are shown in Figure 3.5 (a) to (c).

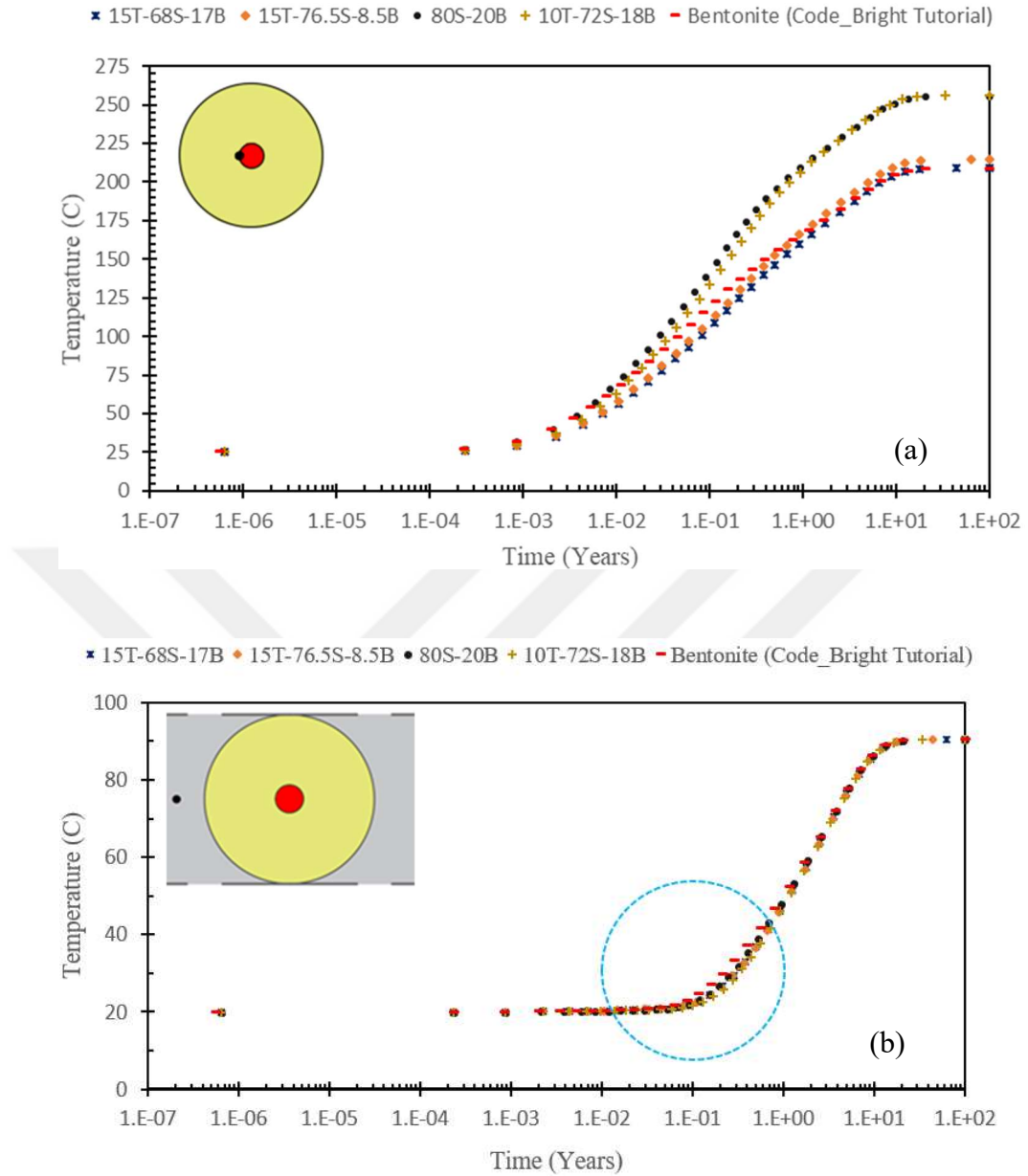


Figure 3.5 The graph of temperature versus time by using 5 different materials: (a) at node [29.5;30.0], (b) at node [26.0;30.0], (c) magnified shape of the region indicated by the blue circle at Figure 3.5 (b)

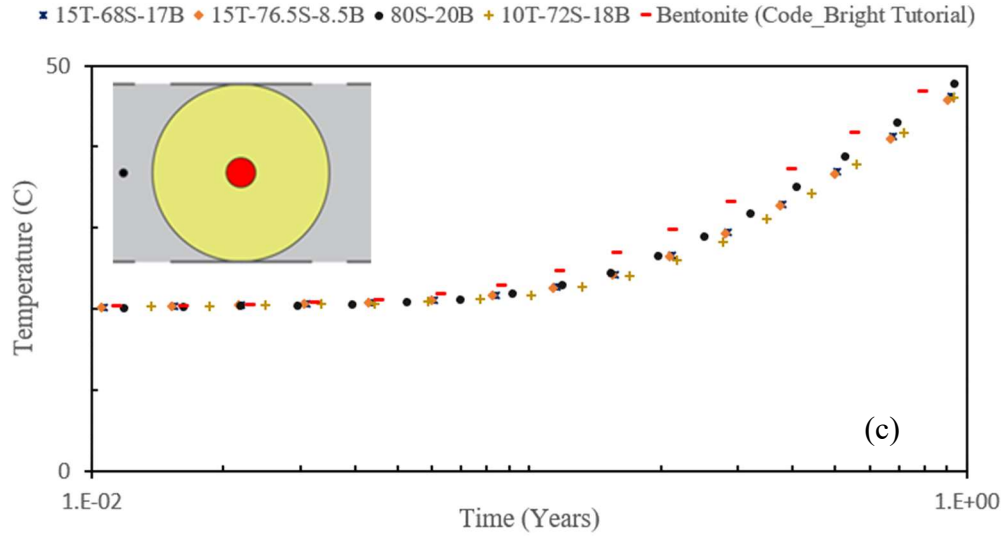


Figure 3.5 continues

As seen in Figure 3.5 (a), because there was about a 57% difference between the volumetric heat capacity of the 15T-68S-17B boron-added mixture and that of the bentonite (CODE_BRIGTH Tutorial) material, the canister surface heated up faster in the model using the bentonite (CODE_BRIGTH Tutorial) material. On the other hand, because the thermal conductivity coefficients of 15T-68S-17B and bentonite (CODE_BRIGTH Tutorial) materials were the same, the final temperatures on the canister surface after 100 years were almost equal to each other, being around 209°C. A similar situation was also observed in the models constructed using 80S-20B and 10T-72S-18B (Figure 3.5 (a)).

The temperature of the canister surface in the model with 10T-72S-18B started to increase lately than the model with 80S-20B. The canister surface temperatures obtained after 100 years were about 256°C and 255°C for the models with 10T-72S-18B and 80S-20B, respectively. An approximate 1°C temperature difference is due to the thermal conductivity coefficient difference between the two materials. When evaluating the analysis results of models constructed using 15T-76.5S-8.5B and 15T-68S-17B materials, because the heat storage capacities of both materials were almost the same, their temperatures increased at the same rate over the time periods; however, the final temperatures on the canister surface were different due to their different thermal conductivity coefficients. In the FEM model with 15T-76.5S-8.5B, the

canister surface had a temperature of 214.5°C after 100 years while the final canister surface temperature was 209°C in the model with 15T-68S-17B.

Examining Figure 3.5 (b) and (c), because the heat diffusion rate for the bentonite (CODE_BRIGHT Tutorial) material was higher compared to other samples, the temperature at the point outside the buffer layer increased in a short time. Moreover, because the material with the lowest heat diffusion rate was 10T-72S-18B, the temperature increase at the point with coordinates of [26.0,30.0] outside the buffer was observed later. For these reasons, it can be said that thermal conductivity and volumetric heat capacity values of a material should be considered when selecting and evaluating candidate materials that will be in contact with the canister and the buffer materials to be used around the canister.

It can be seen from the analysis results that a 47°C temperature increase can be observed on the canister surface after 100 years depending on the thermal conductivity coefficients of the materials.

Volumetric heat capacity values play an important role in the heat transfer mechanism in 0 to 12 years short-term analyses. Thus, it is necessary to examine sudden temperature increases in the material with short-time analyses and the associated mechanical and hydraulic parameter changes in detail. On the other hand, for long-term analyses, basically, the thermal conductivity coefficient is important. All these deductions were made in situations where heat flux was kept constant, as given in the CODE_BRIGHT Tutorial-Thermal problem (2019). In the analyses performed to simulate the situation closest to reality, the heat flux value was gradually decreased depending on the radioactive half-life of the substances and BCs defined in the related model. As a result of analyses made for BCs where the amount of heat energy generated by spent fuel will decrease with respect to time, it is obvious that the canister surface temperature will reach its peak and decrease with time.

To determine the roles of thermal conductivity coefficient, volumetric heat capacity and heat diffusion rate on the partial differential equation defining heat transfer more

comprehensively, the geometry in Figure 3.1, all BCs given in the CODE_BRIGHT Tutorial-Thermal problem (2019) and the material types were kept the same, the density value of bentonite in the tutorial (2000 kg/m^3) was decreased to 1500, 1000 and 500 kg/m^3 and the volumetric heat capacity ($\rho.c_p$) values were decreased from $2.0\text{E}+06$ to $1.5\text{E}+06$, $1.0\text{E}+06$ and $0.5\text{E}+06 \text{ J/m}^3\text{-K}$, respectively –keeping the thermal conductivity coefficient and specific heat constant. The temperature–time graphs for a point with coordinates $[29.5;30.0]$ on the canister surface and a point with coordinates $[26.0;30.0]$ in the host rock were obtained and are given in Figure 3.6 (a) to (c).

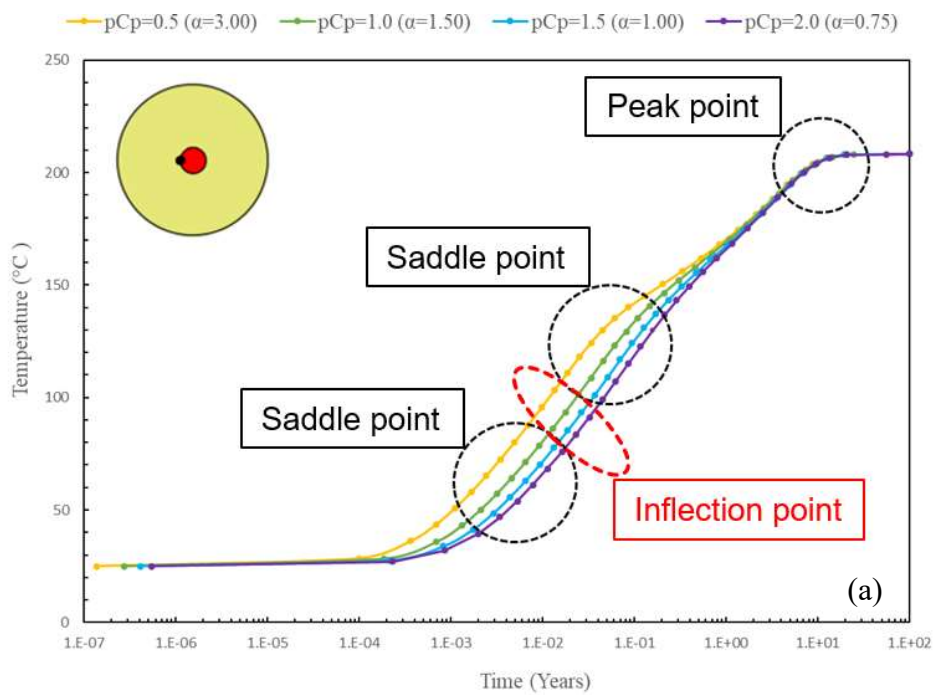


Figure 3.6 The graph of temperature versus time: (a) at node $[29.5;30.0]$, (b) at node $[26.0;30.0]$, (c) magnified shape of the region indicated by the blue circle at Figure 3.6 (b)

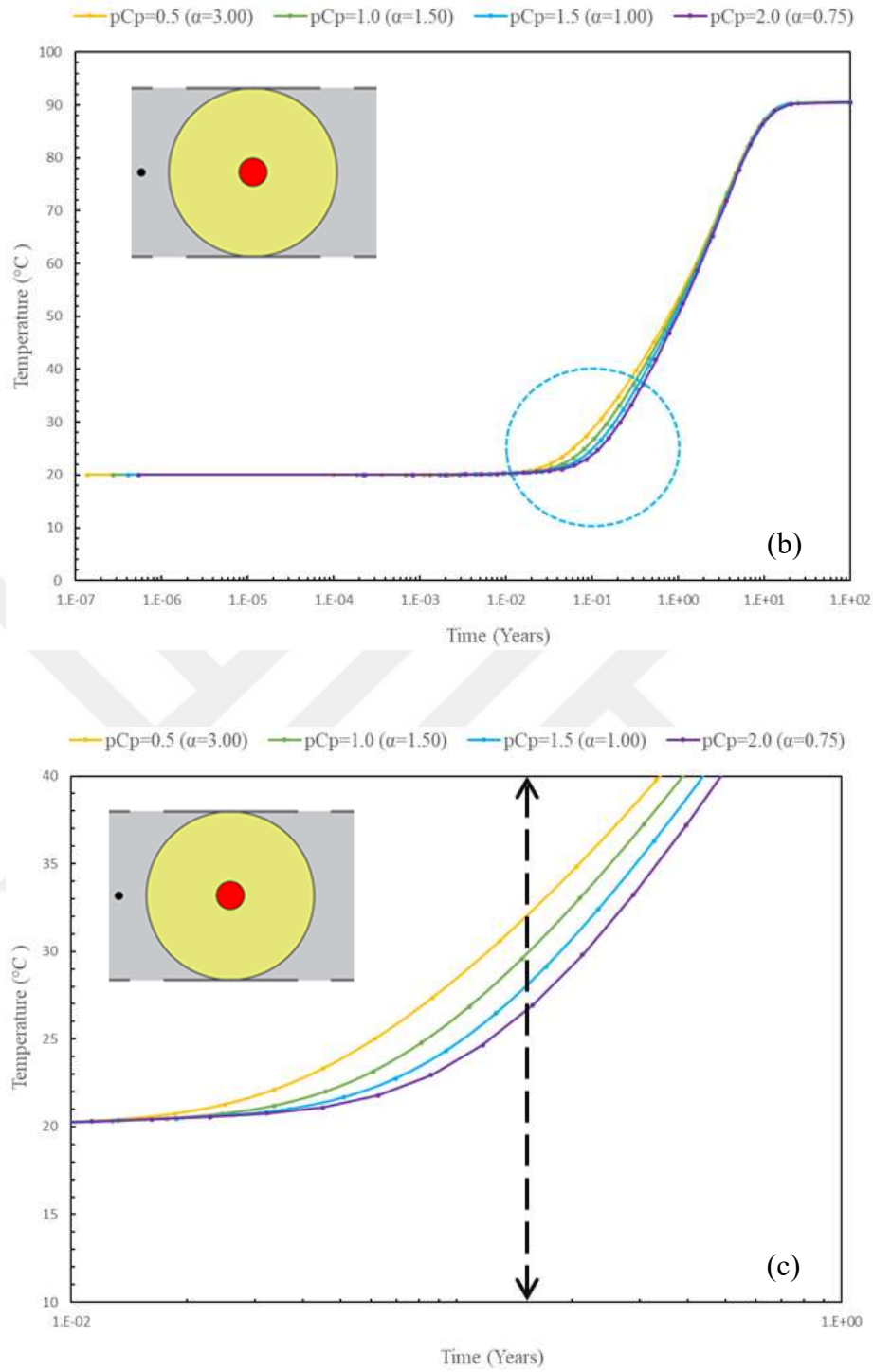


Figure 3.6 continues

It is seen from Figure 3.6 (a) that the canister surface temperature increases later as the volumetric heat capacity of bentonite rises. On the other hand, in the model constructed using the sample with the highest volumetric heat capacity, it can be seen from Figure 3.6 (b) and (c) that because the sample's heat diffusion coefficient is low,

the temperature at the point with coordinates [26.0;30.0] in the host rock starts increasing later. Because the heat diffusion rate increased due to decreased volumetric heat capacity, the heat generated by the nuclear waste was transferred from the buffer layer to the host rock layer faster. On the other hand, because the thermal conductivity coefficient was equal for all samples, the final temperature value was 208.2°C.

As a result, when heat energy diffusion is realized by conduction, the material parameters (λ_f , c_p and p) that are dominant in the transfer mechanism and present in the partial differential equations, determine the coordinates of the saddle and the peak points of a specified point on the temperature–time curve. Thermal conductivity coefficient and volumetric heat capacity are significant parameters for the canister surface, while heat diffusion coefficient is important for the rock layer. For all these reasons, the analysis time is a very important issue in engineering problems based on the heat transfer mechanism.

3.2 Factors Affecting Thermal Conductivity

As mentioned in the introduction section, it is known that the three factors affecting thermal conductivity coefficient values the most are density, water content and void ratio. In addition to these factors, the fine particles content and organic matter content are other important factors affecting thermal conductivity. Therefore, the focus was on how much the aforementioned material characteristics changed the thermal conductivity and the results obtained are shown in Figures 3.7 to 3.10.

As can be seen from Figure 3.7 (a) and (b), the thermal conductivity coefficient increases with increasing amounts of boron additives. The reason for this is that the thermal conductivity coefficients of porous materials are related to the amount of fine particles. This is because 5%, 10% and 15% boron additives increase the amount of fine particles in the total mixture of solid material. A possible reason for this is that the decrease in the amount of bentonite is lower than the increase in the amount of boron. In other words, the amount of decrease in bentonite was 0.5% in the first group and 1% in the second group, while the amount of increase in boron was 5% in both

sample groups. Thus, the total increase in the amount of fine particles in each increment was 4.5% in the first group and 4% in the second group samples. In the 10% bentonite group, the amount of fine particles increased from 10% to 14.5%, 19% and 23.5%, depending on the amount of boron additives; in comparison with the sample group with 20% bentonite, it increased from 20% to 24%, 28% and 32%.

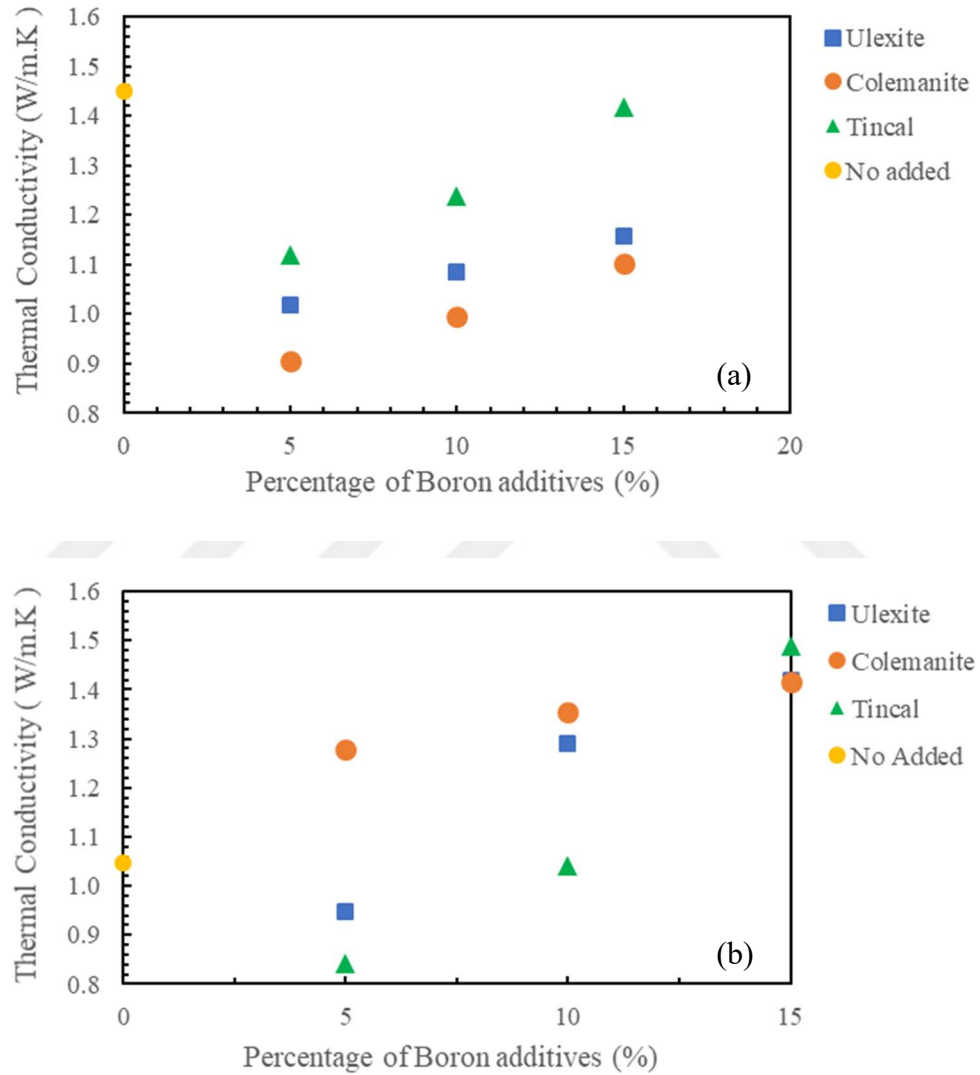


Figure 3.7 (a) Boron added to 10% bentonite, (b) Boron added to 20% bentonite

The graph including all samples constructed by using percentages of fine particles and thermal conductivity values are given in Figure 3.8.

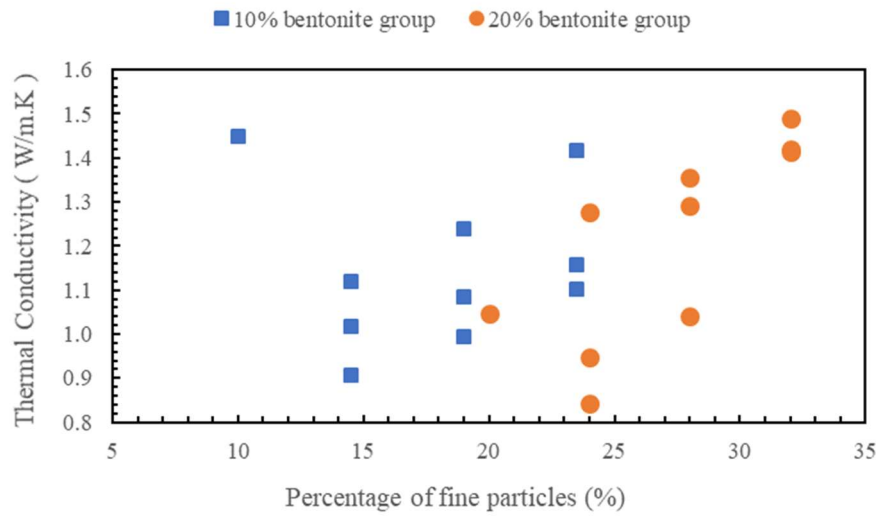


Figure 3.8 Percentage of fine particle content for each of the samples

It can be seen from Figure 3.8 that the thermal conductivity value has an increasing trend with an increasing amount of fine particles. However, it was determined from the 10% bentonite group that when the percentage of fine particles increased from 10% to 14.5%, the thermal conductivity decreased; when it increased from 14.5% to 19% and 23.5%, the thermal conductivity increased. In the first group of samples with 5% boron additives, the decrease in the thermal conductivity was due to the fact that the thermal conductivity value for the boron mineral was very low compared to that of bentonite. The reason for the increases in the thermal conductivities of samples in the first group, despite 10% and 15% boron additives, was thought to be the fact that the effect of the increase in the amount of fine particles on thermal conductivity value was larger than the effect caused by the boron additive. In the samples of the second group, the fine particle effect was not as significant. By contrast, the reason why the same effect was less than in the first group of samples was the increase in the water content of the samples in the second group, which was considered to be an important factor.

Increases in thermal conductivity values in direct proportion to dry densities were discussed in the previous sections and literature studies were mentioned. In this section, the relationship between the thermal conductivity values of sand–bentonite mixtures with added boron and with dry density values was analyzed, and the related graphs are shown in Figure 3.9 (a) and (b).

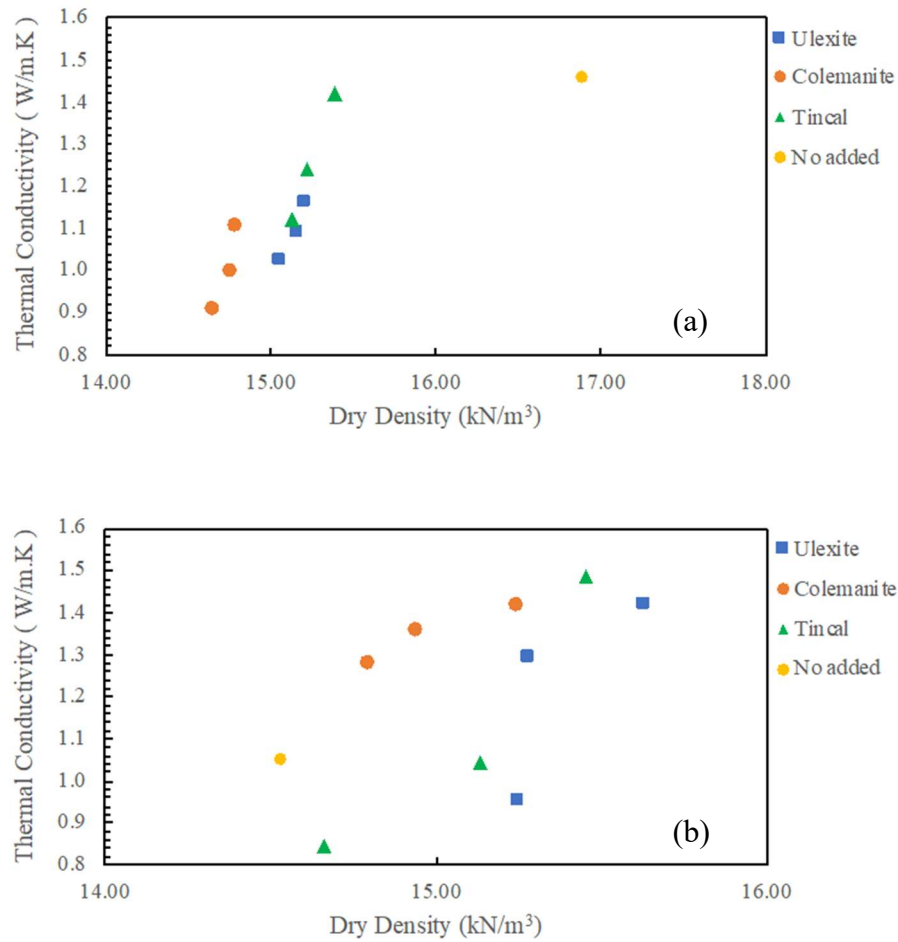


Figure 3.9 Thermal conductivity vs. dry density graphs: (a) Boron added to 10% bentonite mixture, (b) Boron added to 20% bentonite mixture

In the sample group with 10% bentonite, the lowest thermal conductivity value was measured in the samples with a dry density of 14.64 kN/m^3 , while the highest value was found in the samples with a dry density of 15.37 kN/m^3 ; in contrast, in the 20% bentonite group, the lowest and highest thermal conductivity values were measured in the samples with a dry density of 15.25 kN/m^3 and 15.46 kN/m^3 , respectively. Considering these density trends, it can be seen from Figure 3.9 (a) and (b) that minor changes in dry densities cause major differences in thermal conductivity values. On the other hand, evaluating the groups in isolation, in terms of boron additive type, it is seen that the thermal conductivity values increase with increasing dry density values in the presence of all boron minerals

A linear increase was found in the first group samples while that linearity was partially seen in the samples with added colemanite and tincal in the second group, but it was not observed in samples with added ulexite. A linear relationship was determined between the dry density and the thermal conductivity coefficient in the first group samples and shown in Equations (3.3), (3.4) and (3.5) for samples with added ulexite, colemanite and tincal, respectively.

$$\lambda_{f,ulexite\ MX} = 0.9156 \delta_{dry,MX} - 12.774 ; R^2 = 0.96 \quad (3.3)$$

$$\lambda_{f,clmnte\ MX} = 1.2304 \delta_{dry,MX} - 17.117 ; R^2 = 0.83 \quad (3.4)$$

$$\lambda_{f,tincal\ MX} = 1.1792 \delta_{dry,MX} - 16.707 ; R^2 = 0.99 \quad (3.5)$$

Thermal conductivity versus optimum water content graphs, including all samples are shown in Figure 3.10. In the sample group with 10% bentonite, the lowest and highest thermal conductivity values were measured at 14.8% and 19.0% for optimum water content, respectively, while in the 20% bentonite group, they were determined to be 16.8% and 20.5% with optimum water content, respectively.

Considering the thermal conductivity changes in terms of optimum water content, it can be seen from Figure 3.10 (a) that, in the first group samples, when water content increased, the thermal conductivity value first decreased to a minimum and then approached that of the additive-free sample. In the second group, it can be seen from Figure 3.10 (b) that the approximate parabolic change observed in the in the samples in the first group was not clearly apparent. It is considered that various factors can result in a non-linear relationship between dry density and optimum water contents in the second group samples, namely increases in the amount of fine particles, changes in water contents, more interaction formed between the increase in the amount of bentonite and anions or cations in the boron, and porous mixtures with fine particles that have an optimum amount of material in terms of thermal conductivity and exceed these values. On the other hand, it is considered that material optimization – where sand–bentonite mixtures with added boron have the lowest thermal conductivity

values – has a particular water content value, dry density value and amount of fine particles.

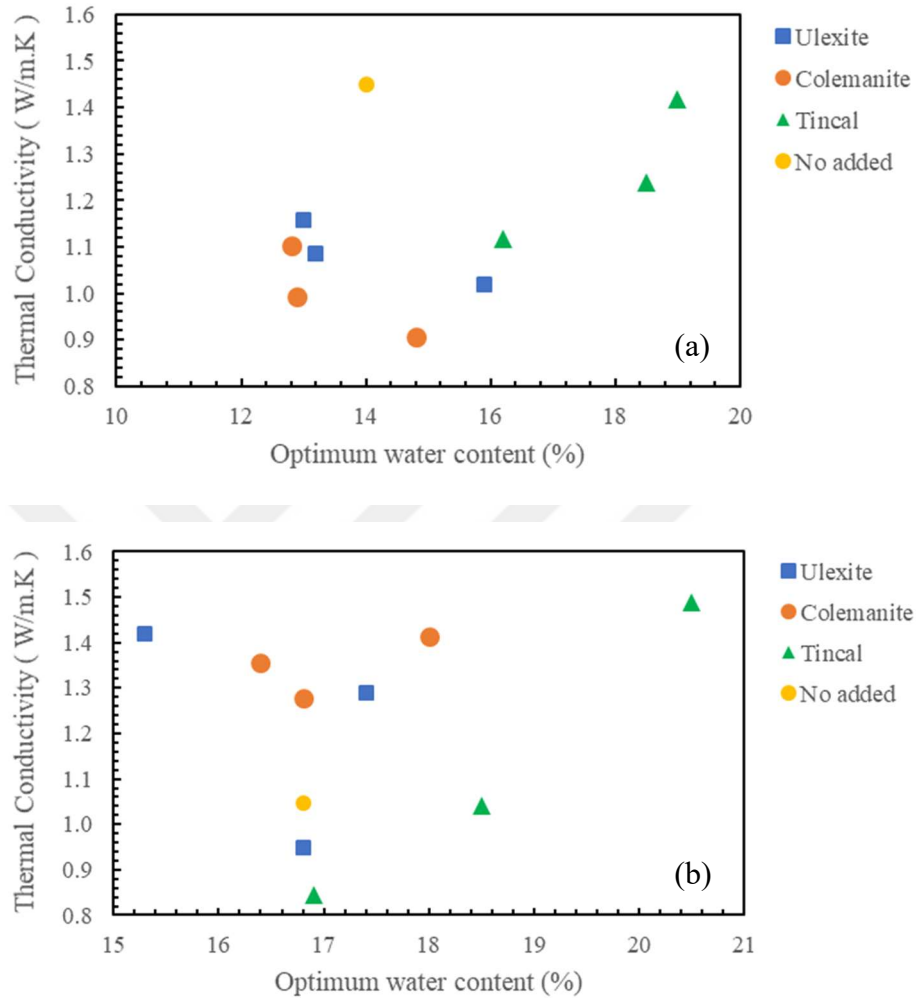


Figure 3.10 Thermal conductivity vs. optimum water content graphs: (a) Bentonite mixture with 10% added Boron (b) Bentonite mixture with 20% added Boron

To analyze possible optimum values, the additive type and percentage, dry density values, optimum water content and percentages of fine particles of the samples, including the lowest and highest thermal conductivity values measured in 10% and 20% bentonite mixtures, are shown in Table 3.12.

Table 3.12 Minimum and maximum thermal conductivity values of 10% and 20% bentonite mixtures

Type	10% Bentonite			20% Bentonite		
	Ref ₁₀	Min ₁₀	Max ₁₀	Ref ₂₀	Min ₂₀	Max ₂₀
Composite	90S-10B	5C-85.5S-9.5B	15T-76.5S-8.5B	80S-20B	5T-76S-19B	15T-68S-17B
Boron (%)	0.00	5.00	15.00	0.00	5.00	15.00
λ_f (W/m-K)	1.450	0.906	1.417	1.048	0.844	1.489
δ_{dry} (kN/m ³)	16.89	14.64	15.37	14.54	14.66	15.46
ω_{opt} (%)	14.00	14.80	19.00	16.80	16.90	20.50
Fine (%)	10.00	14.50	23.50	20.00	24.00	32.00

Examining the limiting values given in Table 3.12, in the 10% bentonite group, the optimum water content and percentage of fine particles of the sample having the minimum thermal conductivity value increased in comparison to the additive-free sample in the same group, but its dry density value decreased. In the 10% bentonite group, the dry density value of the sample with the maximum conductivity value decreased in comparison to the additive-free sample, while its optimum water content and percentage of fine particles increased. When comparing the samples with minimum and maximum conductivity values in the 10% bentonite group, all parameters of the sample with the maximum conductivity value increased in comparison to those of the sample with the minimum conductivity value.

In the 20% bentonite group, all parameters of the samples with minimum and maximum thermal conductivity values increased in comparison to those of the additive-free sample. Comparing the additive-free sample parameters of the two groups, there were decreases in the thermal conductivity value of the second group sample compared to the first group in terms of water content and percentage of fine particles, while the thermal conductivity of the second group samples increased in term of dry density.

3.3 FEM Analysis of Boron-Added Sand-Bentonite Mixtures as a Buffer Rounded HLW Canister by ANSYS

Section 2.3 includes the model analyzed by means of FEM and the model geometry. this chapter presents the analysis results. FEM analyses were performed by

using two different software program packages: CODE_BRIGHT software and the ANSYS 2019R1 Academic software package. CODE_BRIGHT software is a sub-program running in GiD (the personal pre and post processor application). It is very important for researchers studying in this area because it is free-ware and solves geotechnical problem together in terms of THM analyses. In addition, it is used for FEBEX experiments. GiD freely allows meshing up to 1000 elements, while the GiD Developer version does up to 10000 elements.

ANSYS allows free model setup of up to 32000 elements and all analyses performed. The base model and its geometry were investigated within the scope of the PEBS project carried out by EURATOM and the results have been shared with the public periodically. The model examined in this chapter of the study was shared in an official report, “Extrapolation of the models developed for repository long-term evolution and evaluation of uncertainties”. Researchers performed TH (thermo-hydro), THM (thermo-hydro-mechanical) and THO (thermo-osmosis) analyses by defining two different boundary value conditions. In the analyses, for the first BC, the canister surface temperature was kept constant at 100°C for 1000 years, while for the second BC, the heat energy diffuses from the canister surface to its surrounding and thus decreases over time. Because a single-layer buffer was examined in the PEBS report, first this single-layer structure was examined and 15T-68S-17B as a buffer material. Next, double-layer structures were examined. The analyses, the model geometry and information about BCs are given in Table 3.13.

Table 3.13 Analysis type, buffer type and BCs of the model

	Buffer Geometry	Boundary Conditions	Software
Case 1	Single	100°C	ANSYS 2019 R1
Case 2	Single	Heat Flux	ANSYS 2019 R1
Case 3	Double	100°C	ANSYS 2019 R1
Case 4	Double	Heat Flux	ANSYS 2019 R1
Case 5	Single	100°C	CODE_BRIGHT
Case 6	Single	Heat Flux	CODE_BRIGHT
Case 7	Double	100°C	CODE_BRIGHT
Case 8	Double	Heat Flux	CODE_BRIGHT

Figure 3.11 (a) and (b) show the 2D axi-symmetrical (around y-axis) geometry of the $\frac{1}{2}$ model analyzed using FEM with boron-added materials, the regions where they were used and the lines where the BCs were defined.

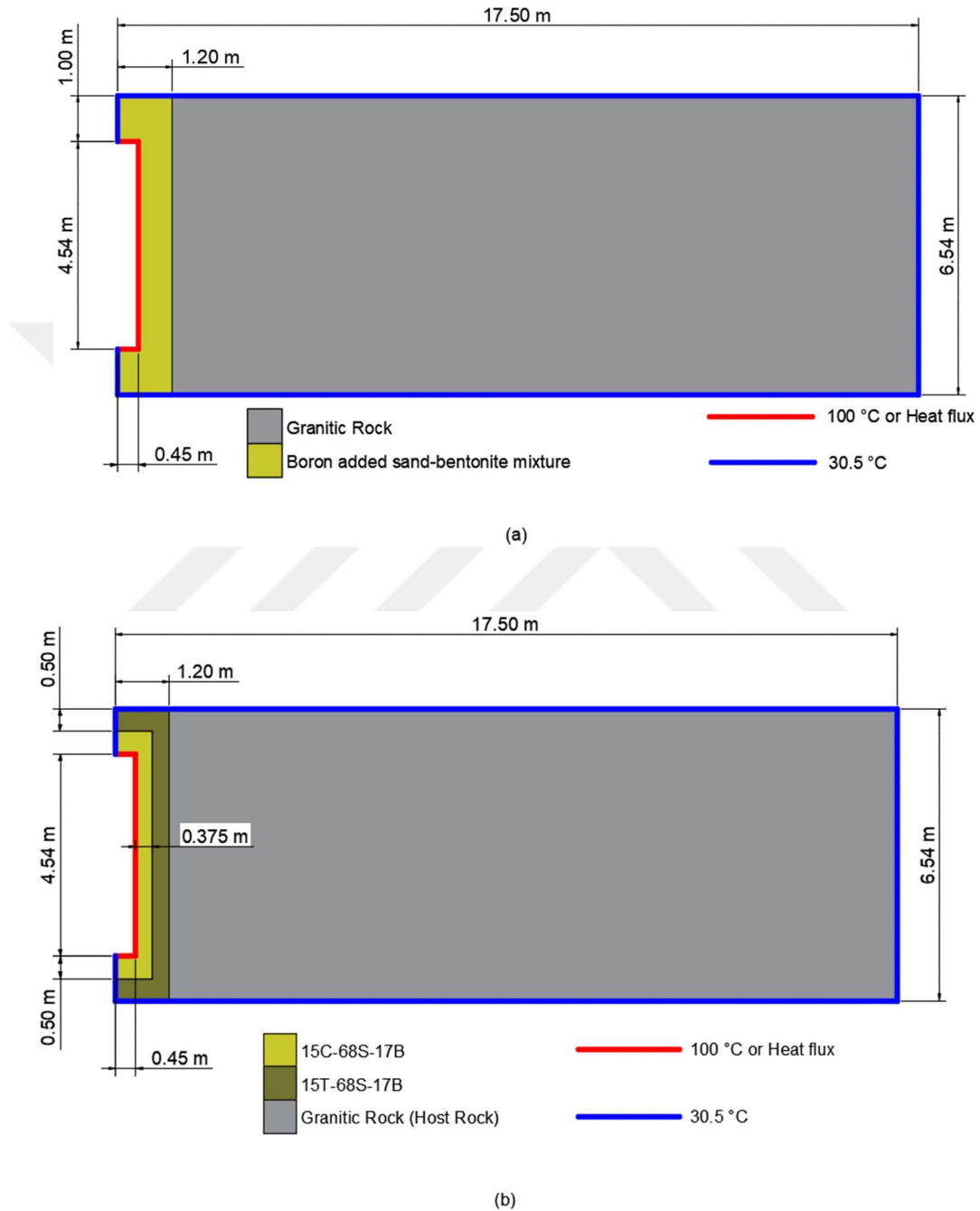


Figure 3.11 The axi-symmetrical (about the y axis) model for FEM analysis: (a) Single-layer buffer, (b) Double-layer buffer

It was mentioned in previous parts that the heat diffusion coefficient and volumetric heat capacity values were significant parameters in short-term analyses, and the materials used in long-term analyses – 1000 years – were basically selected on their thermal conductivity coefficients. The thermal properties of materials used in the model with a single-layer and double-layer buffer are shown in Table 3.14

Table 3.14 The properties of materials used in model

Sample properties		15C-68S-17B	15T-68S-17B	Granitic Rock
S (%)		65.77	75.96	--
e		0.74	0.74	--
ρ (kg/m ³)	Wet	1834	1899	2500
	Dry	1554	1576	2500
λ_f (W/m-K)	Wet	1.415	1.489	3.600
	Dry	0.65	0.65	3.600
c_p (J/kg-K)	Wet	3218	1819	800
	Dry	2583	1111	800
α (m ² /s)	Wet	2.40E-07	4.31E-07	1.80E-06
	Dry	1.62E-07	3.71E-07	1.80E-06

The 15C-68S-17B material was used to decrease the temperature increase on the canister surface and capture radioactive neutron particles, while 15T-68S-17B was used to decrease the temperature increase in the 15C-68S-17B material. Although a minimal temperature increase was expected on the canister surface as a result of constructing all buffer material as a single layer using the 15T-68S-17B mixture, the reason for constructing the buffer as a double layer using 15C-68S-17B in the first layer was that the colemanite mineral would serve as a radioactive barrier. The reason for using 15T-68S-17 as the second layer was to decrease the canister surface with increasing temperature.

Although it does not reflect reality, performing an analysis over a 1000-year time frame by assuming the temperature of the canister surface to be constant at 100°C, it was important to establish reference values. Considering the heat energy generated by spent fuel diffusing from the canister surface to the surroundings as a BC is a more realistic approach. In the PEBS project, heat–time graphs obtained from analyses performed by the CIMNE (International Centre for Numerical Methods in Engineering) research group are shown in Figure 3.12.

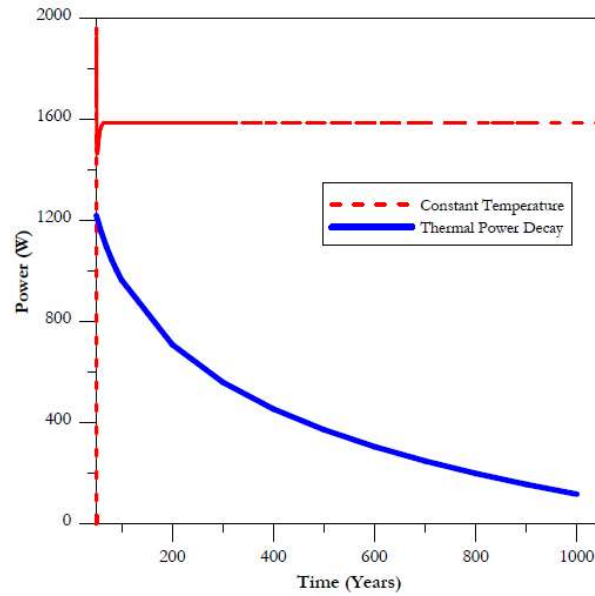


Figure 3.12 Time evolution of the applied thermal power for the case with constant heating temperature and power decay, results up to 1000 year (Wieczorek et al., 2014)

The unit for the y axis in Figure 3.12 is given as Watts. The Watt is known to be Joules/second (J/s). However, one of the most important points to be considered in FEM analyses is that the unit of heat flux is W/m^2 . Therefore, while defining heat flux in the ANSYS software program package, the y axis values in Figure 3.12 need to be divided by the canister surface area (except cylinder bases) (Figure 3.13).

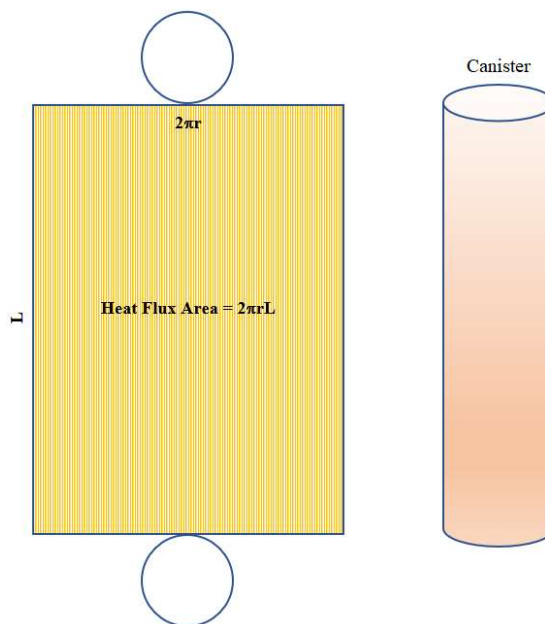


Figure 3.13 Heat flux area and single canister

In this regard, the power decay value needs to be divided by the value of the shaded area (12.837 m^2) shown in Figure 3.13. The power decay (W/canister) graph constructed for use in ANSYS analyses, and the heat flux (W/m^2) values at certain times, are shown in Figure 3.14 and Table 3.15, respectively.

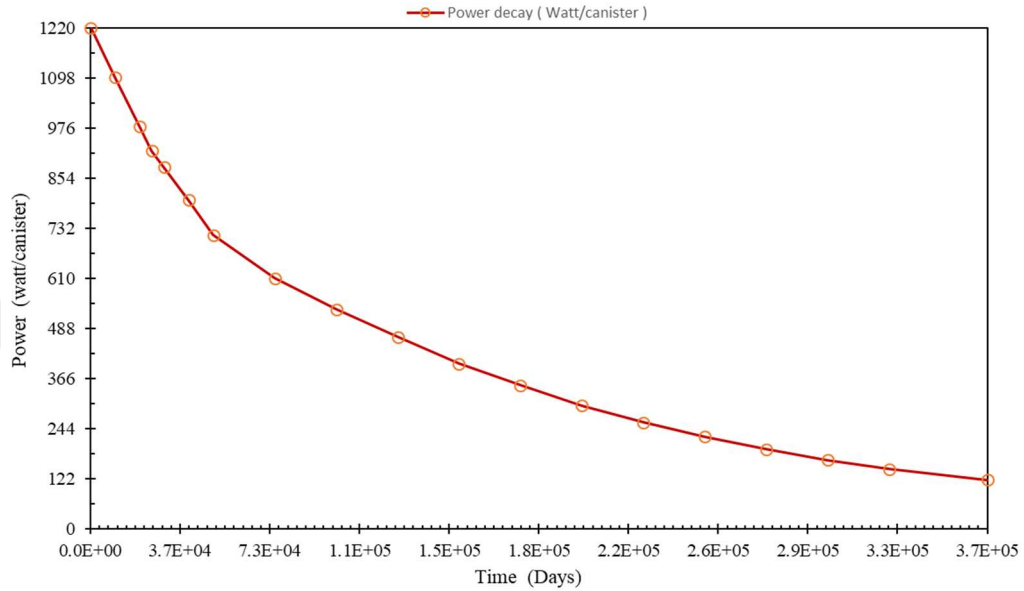


Figure 3.14 Thermal power produced by spent fuel

Table 3.15 The Power Decay and Heat Flux value of nodes given in Figure 3.14

Node	TIME			Power Decay	Heat Flux
	Year	Day	Second	W/canister	W/m^2
1	0.0	0	0.0000E+00	1220	95
2	27.4	10000	8.6400E+08	1100	86
3	54.8	20000	1.7280E+09	980	76
4	68.5	25000	2.1600E+09	920	72
5	82.2	30000	2.5920E+09	880	69
6	109.6	40000	3.4560E+09	800	62
7	137.0	50000	4.3200E+09	715	56
8	205.5	75000	6.4800E+09	610	48
9	274.0	100000	8.6400E+09	535	42
10	342.5	125000	1.0800E+10	467	36
11	411.0	150000	1.2960E+10	402	31
12	479.5	175000	1.5120E+10	350	27
13	547.9	200000	1.7280E+10	300	23
14	616.4	225000	1.9440E+10	260	20
15	684.9	250000	2.1600E+10	225	18
16	753.4	275000	2.3760E+10	194	15
17	821.9	300000	2.5920E+10	168	13
18	890.4	325000	2.8080E+10	146	11
19	1000.0	365000	3.1536E+10	120	9

The values given in Table 3.15 were used to draw only the heat–time graph. In the EUROPAM/PEBS report, the CIMNE research group considered the heat–time graph as a step function. The reason for such a transformation, i.e. the reason for using the heat flux boundary value as a step function is because the CODE_BRIGHT software does not accept BCs as a function or as a tabulated value. Thus, within the scope of this study, Figure 3.15 shows the step function used in the analyses performed with CODE_BRIGHT software with the curvilinear shape given in Figure 3.14.

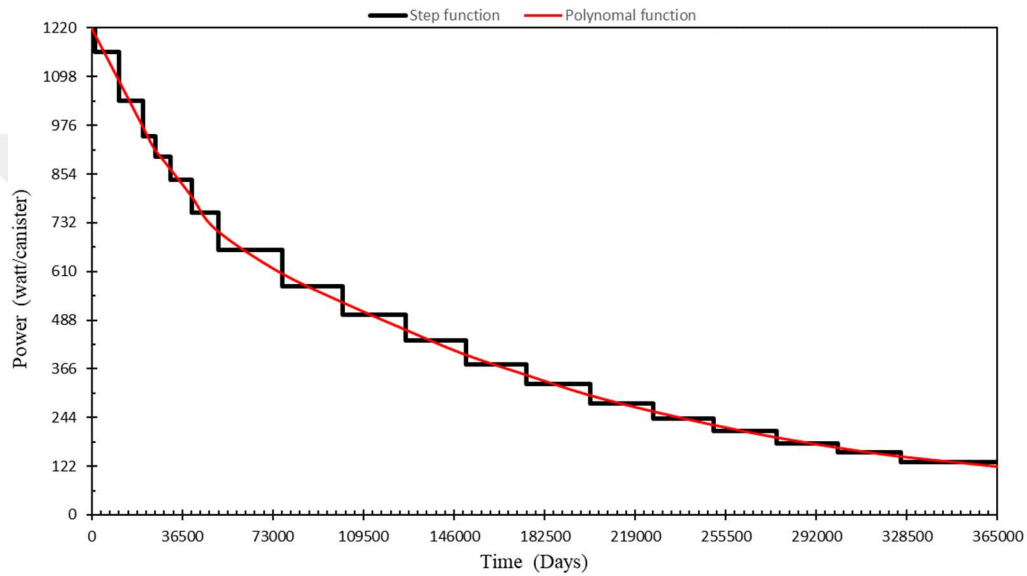


Figure 3.15 Step function of polynomial function of heat source by spent fuel

Initial and end times and the load values of the step function given in Figure 3.15 for each load step are shown in Table 3.16. Presenting initial and end times of the load steps in seconds in Table 3.16 is because the heat flux values are in Watts, i.e. J/s. On the other hand, because the thermal conductivity coefficient (W/m-K) includes Watts, it necessitated the use of seconds as the time unit for ANSYS and CODE_BRIGHT software.

Another concept of the finite elements software is the time step size and substep sizes to be used in calculations. Time step size directly affects the solution sensitivity and total time necessary to arrive at a solution. Therefore, it was concluded that the time step should be 6.3072E+05 s, i.e. 73 days, by using a trial-and-error method for

an optimum solution time over a 1000-year (3.1536×10^{10} s) analysis time; consequently 5000 substeps were formed.

Table 3.16 The Heat flux value of load step given in Figure 3.15

Load Step	Initial Time of Load Step		End Time of Load Step		Power	Heat Flux
	Day	Second	Day	Second	Watt/canister	Watt/m ²
1	0	0.0000000E+00	1215	1.0497600E+08	1220	95
2	1215	1.0497600E+08	10950	9.4608000E+08	1159	90
3	10950	9.4608000E+08	20680	1.7867520E+09	1038	81
4	20680	1.7867520E+09	25550	2.2075200E+09	949	74
5	25550	2.2075200E+09	31630	2.7328320E+09	898	70
6	31630	2.7328320E+09	40150	3.4689600E+09	840	65
7	40150	3.4689600E+09	51110	4.4159040E+09	758	59
8	51110	4.4159040E+09	76650	6.6225600E+09	663	52
9	76650	6.6225600E+09	100980	8.7246720E+09	572	45
10	100980	8.7246720E+09	126530	1.0932192E+10	502	39
11	126530	1.0932192E+10	150865	1.3034736E+10	436	34
12	150865	1.3034736E+10	175200	1.5137280E+10	377	29
13	175200	1.5137280E+10	200750	1.7344800E+10	327	25
14	200750	1.7344800E+10	226300	1.9552320E+10	280	22
15	226300	1.9552320E+10	250630	2.1654432E+10	241	19
16	250630	2.1654432E+10	276180	2.3861952E+10	210	16
17	276180	2.3861952E+10	300515	2.5964496E+10	179	14
18	300515	2.5964496E+10	326065	2.8172016E+10	156	12
19	326065	2.8172016E+10	365000	3.1536000E+10	132	10

Another significant point in the models analyzed using FEM is the mesh concept. Meshing can be done using square or triangular elements, and element densities can be changed with respect to the model geometry. The element type used was PLANE77 (8node 77) for the ANSYS analyses. The mesh model of the geometry given in Figure 3.11 (b) constructed with ANSYS software is shown in Figure 3.16 (a) and (b).

As shown in Figure 3.16 (a), the granite (host rock) area was divided into triangular elements with a 0.5 m unit, while the buffer region around the canister was divided into triangular elements with a 0.05 m unit (Figure 3.16b). Because a nodal solution is obtained by the ANSYS software, temperature values could be obtained at 0.05 m intervals in the buffer region and at 0.5 m intervals in the granite rock region. As a result of constructing the mesh, a total of 12284 nodes and 6503 triangular elements were formed. The mesh concept is also the same in the model with a single-layer buffer.

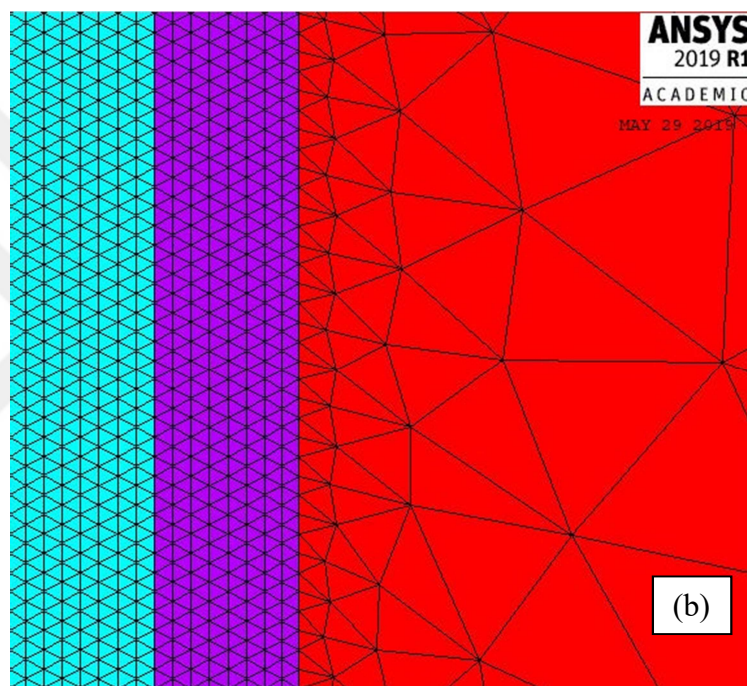
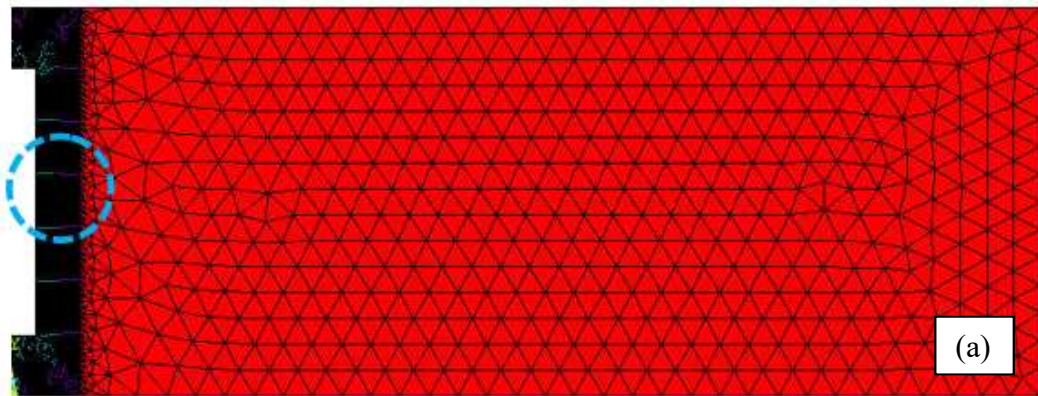


Figure 3.16 The meshing of axi-symmetrical model: (a) all model, (b) area represented by light blue circle shown in Figure 3.17 (a)

The model (Case1) was analyzed using an ANSYS 2019 R1 FEM program over a 1000-year time period under flow BCs where the 15T-68S-17B mixture was used as a single-layer buffer and where the canister surface was kept constant at a temperature of 100°C. Figure 3.17 (a) and (b) shows temperature–time graphs at various points (or nodes) obtained after 1000 years and 15 years, respectively.

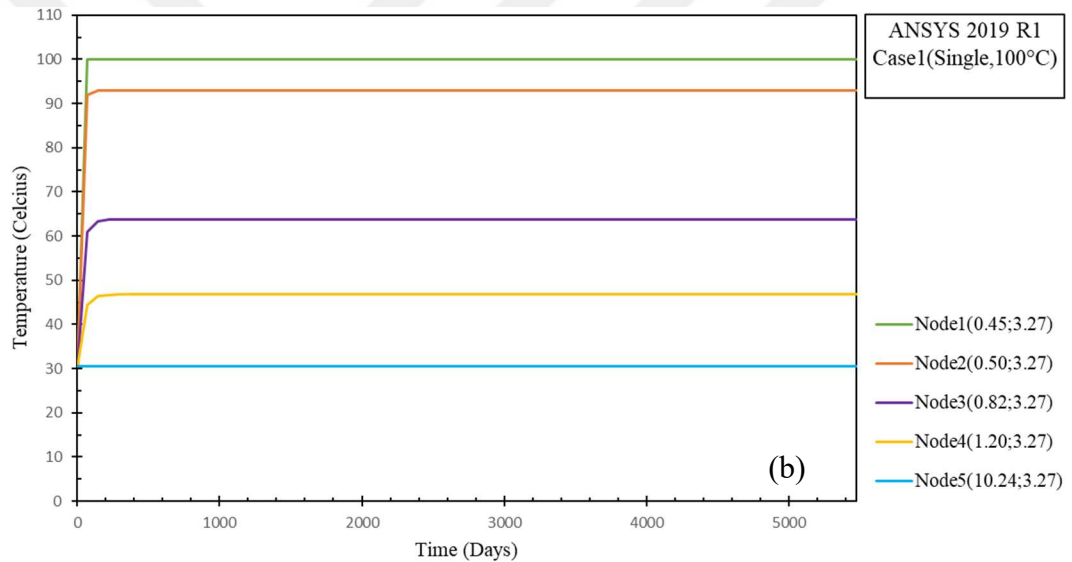
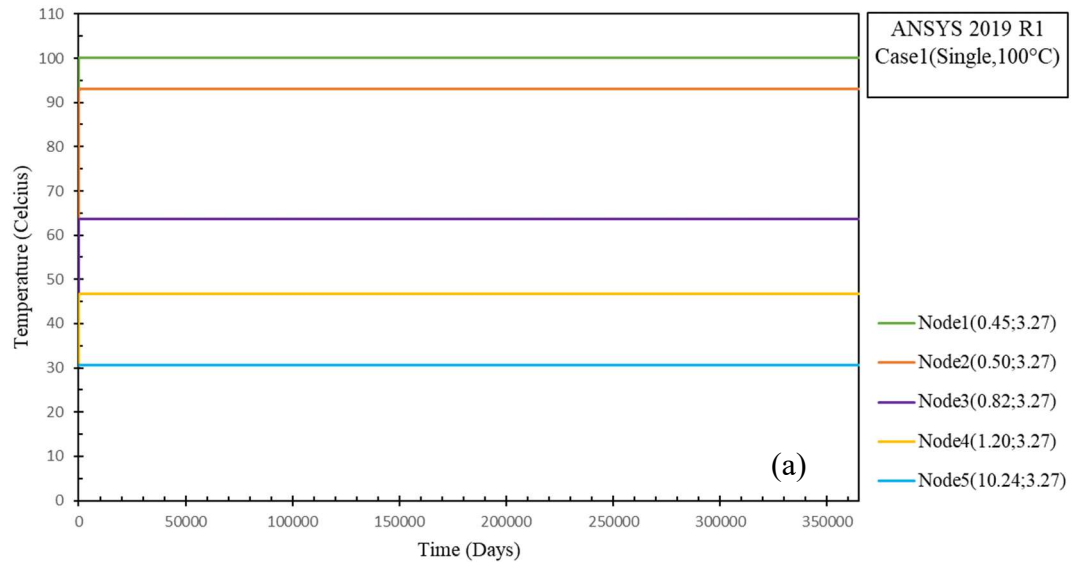


Figure 3.17 The graph of temperature at different positions from the canister has single layer buffer:
(a)Time up to 1000 years, (b)Time up to 15 years

It can be seen from Figure 3.17 (a) that the temperature at Node2, which was 0.05 m away from the canister surface, was approximately 93°C. Moreover, the temperatures at Node3 and Node4, which were 0.37 m and 0.75 m away from the canister surface, were calculated to be 64°C and 47°C, respectively. The temperature at Node5, which was inside the rock and approximately 9.79 m away from the canister surface, was 31°C after the 1000-year analysis time. It can be seen from Figure 3.17 (b) that the temperature at all nodes reached a steady state after approximately 180 days.

Nonlinear analysis (thermal conductivity changes depending on temperature) of the model (Case2) where the 15T-68S-17B mixture was used with a single-layer buffer, and the BC represented heat flux diffusing from the canister surface, was performed by the ANSYS 2019 R1 FEM program. Figure 3.18 (a) and (b) shows the analysis results for a 1000-year and 15-year time period, respectively.

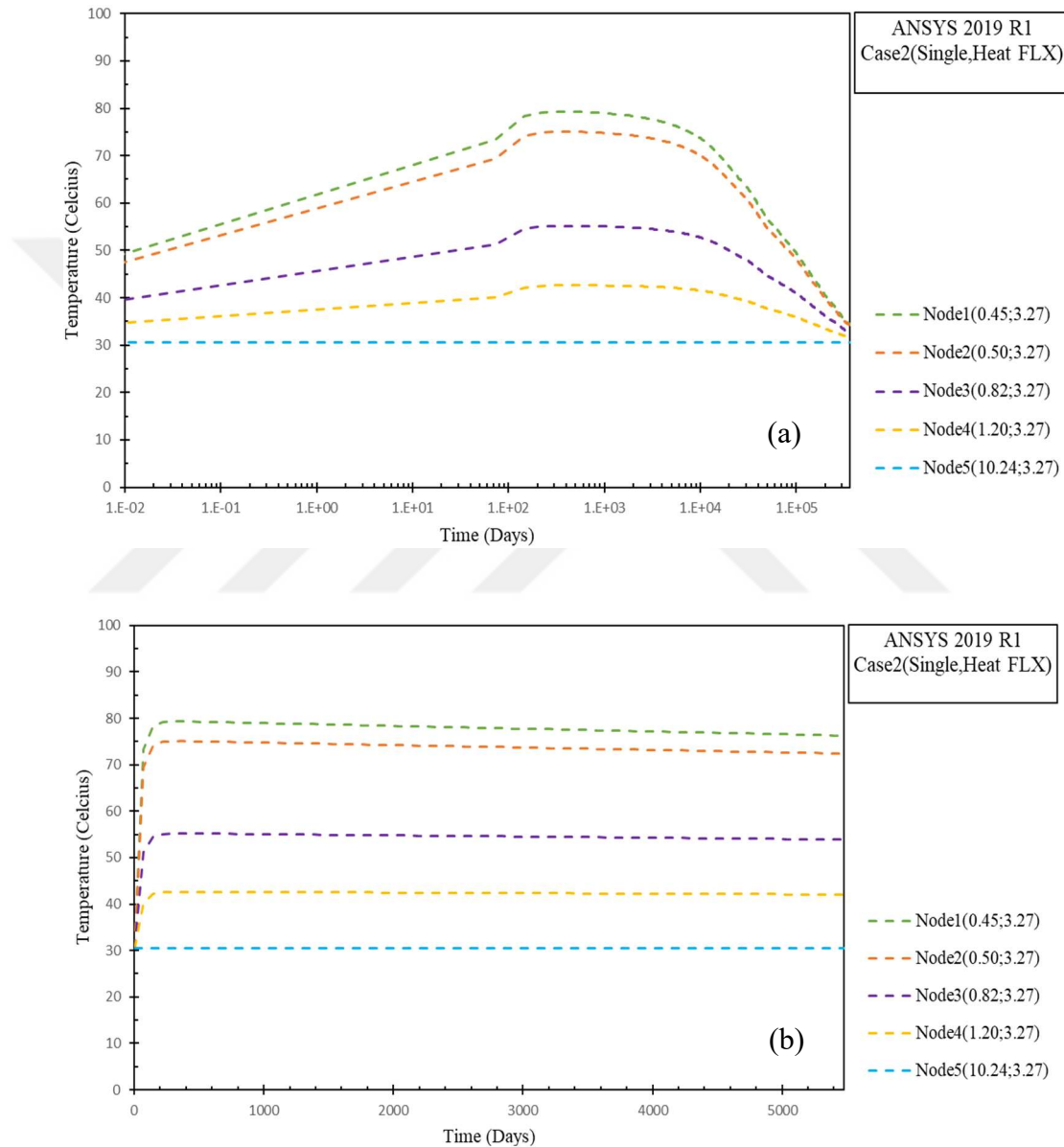


Figure 3.18 The graph of temperature at different positions from canister has single layer buffer by using heat flux boundary conditions: (a)Time up to 1000 years, (b)Time up to 15 years

As a result of analyses for Case2 conditions, the maximum temperature at Node1 on the canister surface was 79°C. In addition, the temperatures of Node2, Node3 and

Node4, which were 0.05 m, 0.37 m and 0.75 m away from the canister surface, were found to be approximately 75°C, 55°C and 43°C after 1000 years, respectively. The temperature at Node5, which was inside the rock and approximately 9.76 m away from the canister surface, was 31°C after the 1000-year analysis time. In addition to Case1 and Case2, whose analysis results are presented above, models Case3 and Case4 with the double-layer buffer design used with two different flow BCs were analyzed using the ANSYS 2019 R1 package program. Figure 3.19 (a) and (b) shows the analysis results of the model Case3 – where a canister surface temperature of 100°C was used as the flow BC – obtained after a 1000-year and 15-year time period, respectively.

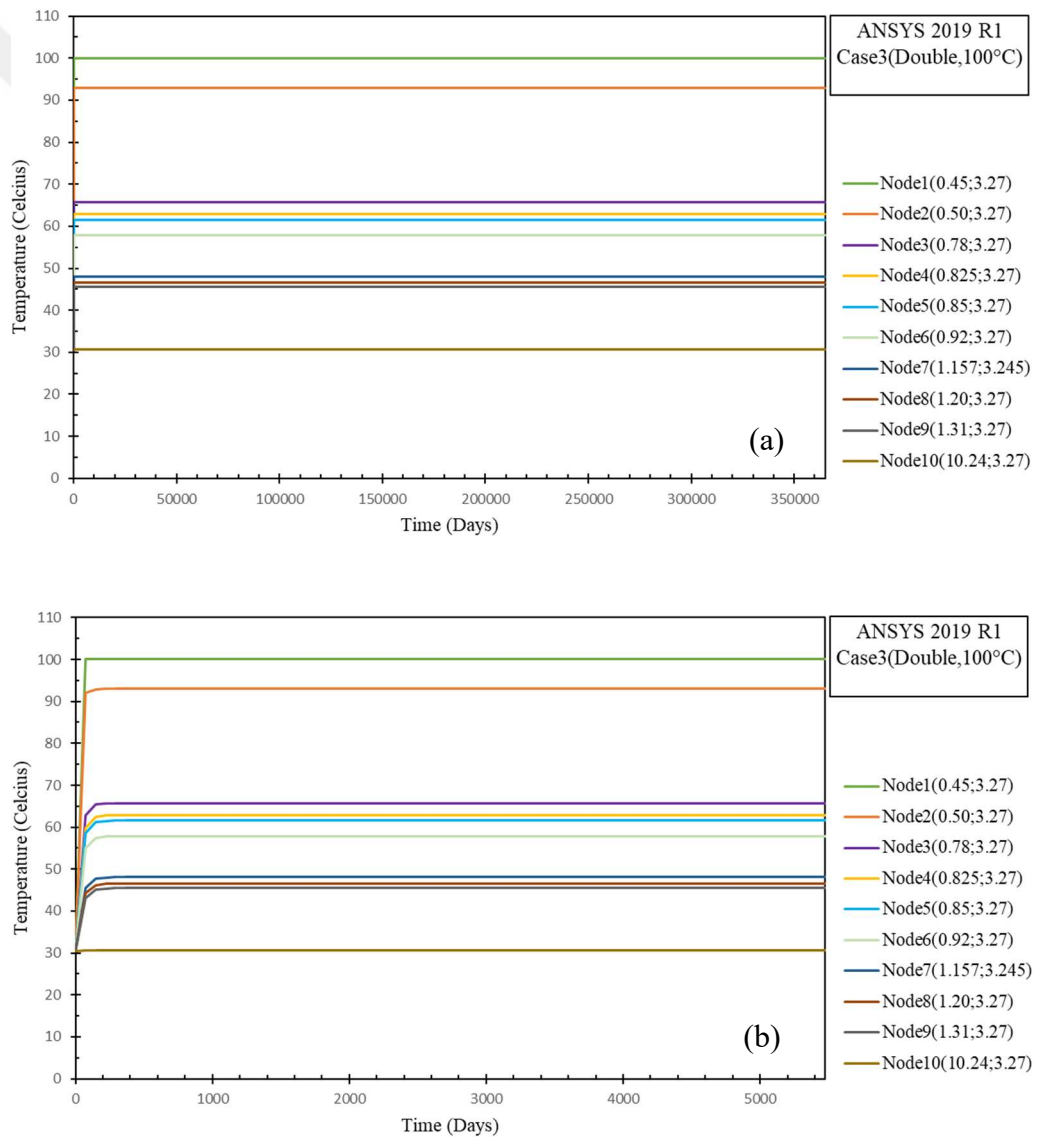


Figure 3.19 The graph of temperature at different positions from canister has double layer buffer: (a)Time up to 1000 years, (b)Time up to 15 years

It can be seen from Figure 3.19 (a) that the temperature of the canister surface was kept constant at 100°C due to the boundary condition, the temperature at Node2, which was 0.05 m away from the canister surface, was approximately 93°C. The temperatures of Node3, which was 0.33 m away from the canister surface, and Node4, which was at the intersection of two layers and 0.375 m away from the canister surface, were calculated to be 66°C and 63°C, respectively. The temperatures at Node5, Node6 and Node7 inside the second buffer layer were found to be 62°C, 58°C and 48°C after 1000 years. The temperature at Node8, which was at the buffer–host rock interface, was 47°C. The temperatures of Node9, which was 0.86 m away from the canister surface, and Node10, which was 9.79 m away from the canister surface, were almost equal to each other (31°C) after the 1000-year analysis time. It can be seen from Figure 3.19 (b) that all nodes reached a steady state after approximately 180 days.

Figure 3.20 (a) and (b) shows the analysis results of the model Case4 designed with a double buffer, where heat flux was used as the flow BC over a 1000-year and 15-year time period, respectively. It can be observed from Figure 3.20 (a) that the temperature of the node on the canister surface first reached 80°C and then decreased down to 35°C after 1000 years. The temperature at Node2, which was 0.05 m away from the canister surface, increased to 76°C and then decreased down to 34°C after 1000 years. Temperatures of two nodes – one of them, Node3, at the intersection of two layers and 0.33 m away from the canister surface and the other, Node4, 0.375 m away from the canister surface – were calculated to be approximately 57°C and 55°C, respectively. Temperatures of nodes 5, 6 and 7, which were inside the 15T-68S-17B second-buffer layer, were found to be 54°C, 51°C and 44°C, respectively. The maximum temperature of Node8, which was at the buffer–host rock intersection, was calculated to be 43°C. The temperatures of two nodes inside the rock – one of them, Node9, 0.86 m away from the canister surface and the other, Node10, 9.79 m away – were calculated to be approximately 42°C and 31°C, respectively. It is seen from Figure 3.20 (a) and (b) that temperature reached a peak value after 200 days for all nodes and decreased over time, being less than 40°C after 1000 years.

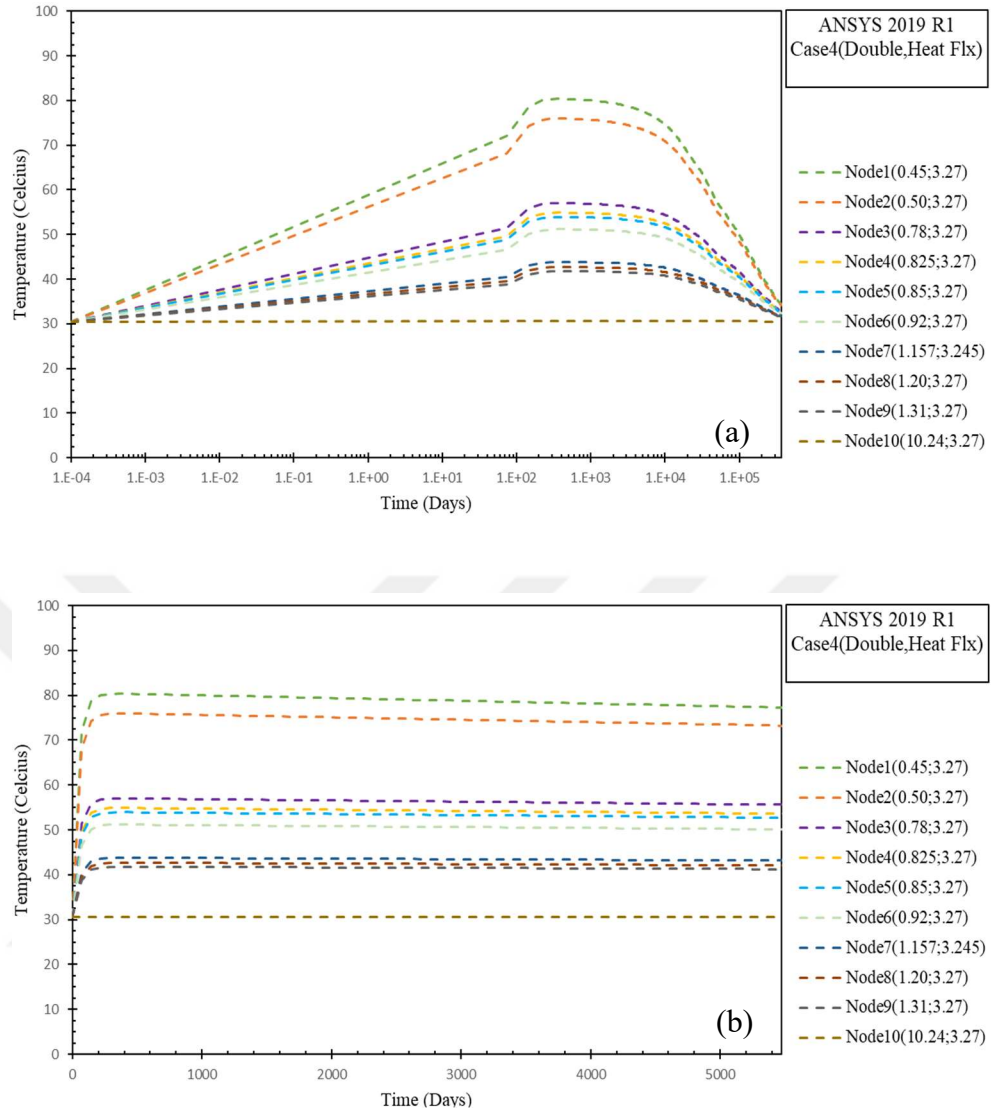


Figure 3.20 The graph of temperature at different positions from canister has double layer buffer by using heat flux boundary conditions: (a)Time up to 1000 years, (b)Time up to 15 years

3.4 FEM Analysis of Boron-Added Sand-Bentonite Mixtures as a Buffer Rounded HLW Canister by CODE_BRIGHT

In the previous section, thermal analyses of the model given in Figure 3.11 (a) and (b) were performed using the ANSYS 2019 R1 program, and in this section, the same model was analyzed by GiD and CODE_BRIGHT software using the same BCs.

In CODE_BRIGHT software, although values can be input for λ_{dry} and λ_{wet} , the program performs its solution using λ_{wet} . This is because the program calculates the

thermal conductivity coefficient according to degree of saturation. Because the solution obtained using this method is a Thermo-Hydro process, within the scope of this study, the hydro part was not analyzed by the program. For these reasons, the thermal conductivity coefficients of 15C-68S-17B and 15T-68S-17B mixtures, which were used as buffers, were included by averaging the λ_{dry} and λ_{wet} values (Min, L., & Avin, C. K. L., 2015).

The analysis results obtained using CODE_BRIGHT software were found to be very close to those obtained by using the ANSYS 2019 R1 program. Figure 3.21 (a) and (b) shows the analysis results of the model Case5 designed as a single-layer buffer using 15T-68S-17B, where the temperature of the canister surface for flow BCs was constant at 100°C.

It is seen from Figure 3.21 (a) that the temperature of node2, which was 0.05 m away from the canister surface, was around 93°C. Temperatures of Node3 and Node4, which were 0.37 m and 0.75 m away from the canister surface, were calculated to be 67°C and 48°C after the 1000-year analysis time, respectively. The temperature of Node5, which was inside the rock and 9.79 m away from the canister surface, was 31°C after the 1000-year analysis time. It can be seen from Figure 3.21 (b) that the temperature at all nodes reached a steady-state value after about 30 days.

The model Case6, where the 15T-68S-17B mixture was used as a single-layer buffer and where the BC was heat flux diffusing from the canister surface, was analyzed by CODE_BRIGHT software, and Figure 3.22 (a) and (b) shows results for a 1000-year and 15-year time period, respectively.

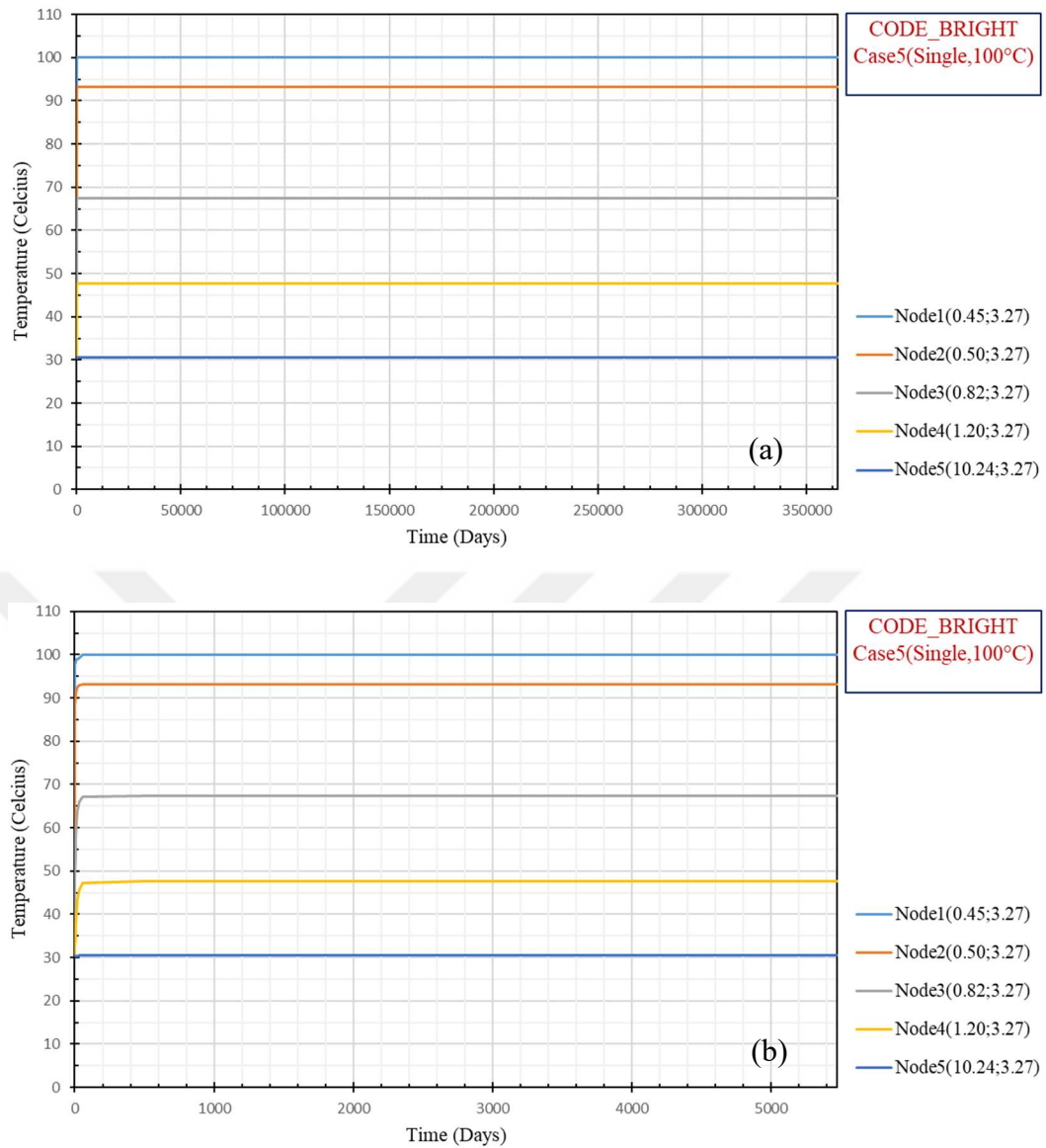


Figure 3.21 The graph of temperature at different positions from the canister has single layer buffer analysis by CODE_BRIGHT: (a)Time up to 1000 years, (b)Time up to 15 years

As a result of analyses performed with Case6 inputs, the temperature of Node1 on the canister surface was found to be 81°C. In addition, the temperatures of Node2, Node3 and Node4, which were 0.05 m, 0.37 m and 0.75 m away from the canister surface, were approximately 77°C, 57°C and 43°C after 1000 years, respectively. The temperature of Node5, which was inside the rock and 9.76 m away from the canister surface, was around 31°C after 1000 years.

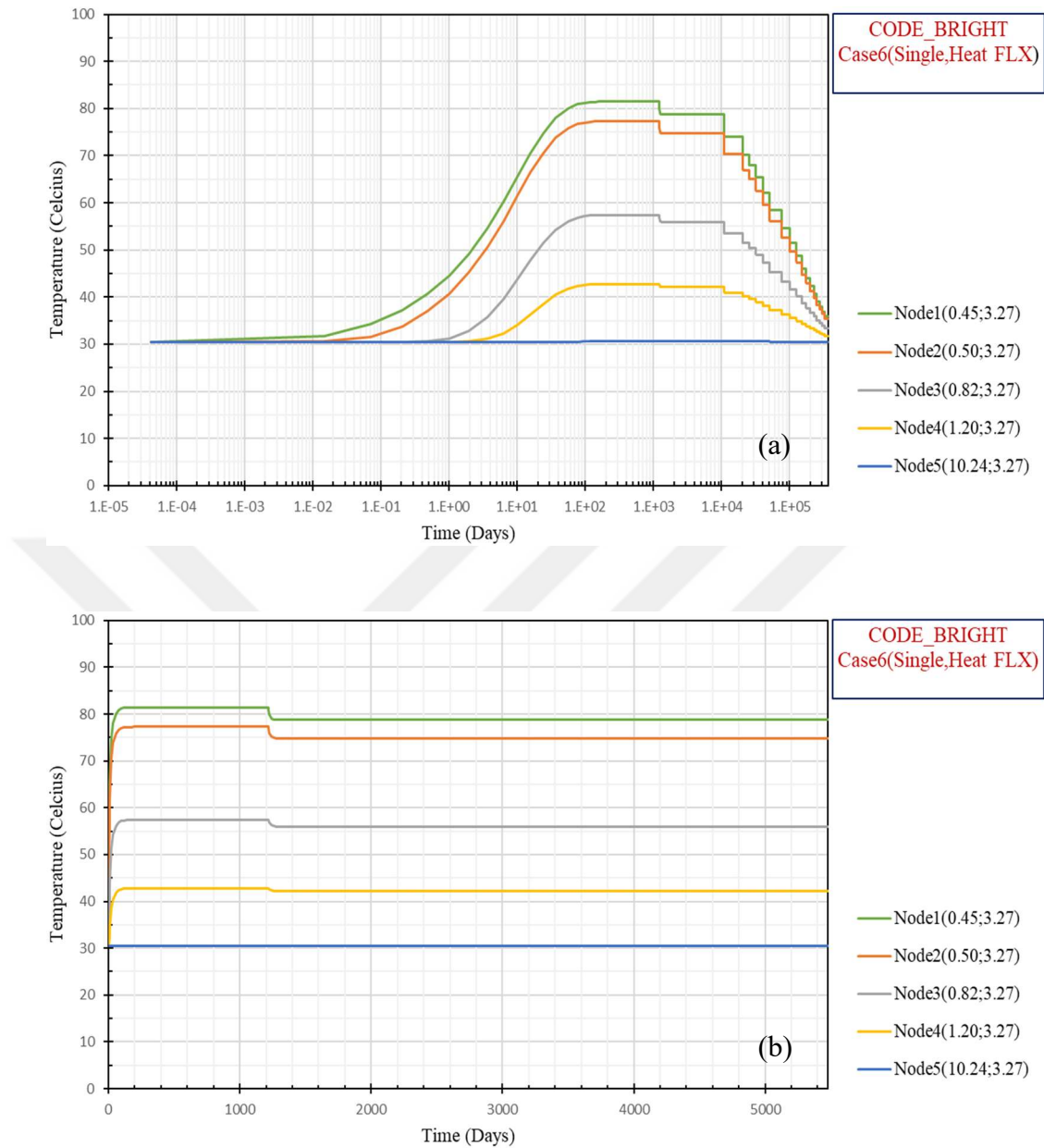


Figure 3.22 The graph of temperature at different positions from canister has single layer buffer by using heat flux boundary conditions analysis by CODE_BRIGHT: (a)Time up to 1000 years, (b)Time up to 15 years

Analysis results for Case7 (Single layer – 100°C) and Case8 (Single layer – Heat Flux) models using CODE_BRIGHT software are shown in Figures 3.23 and 3.24. In this section, the analysis results for Case7 designed with a double layer, where the flow BC was a 100°C canister surface temperature, after a 1000-year and 15-year period, are shown in Figure 3.23 (a) and (b).

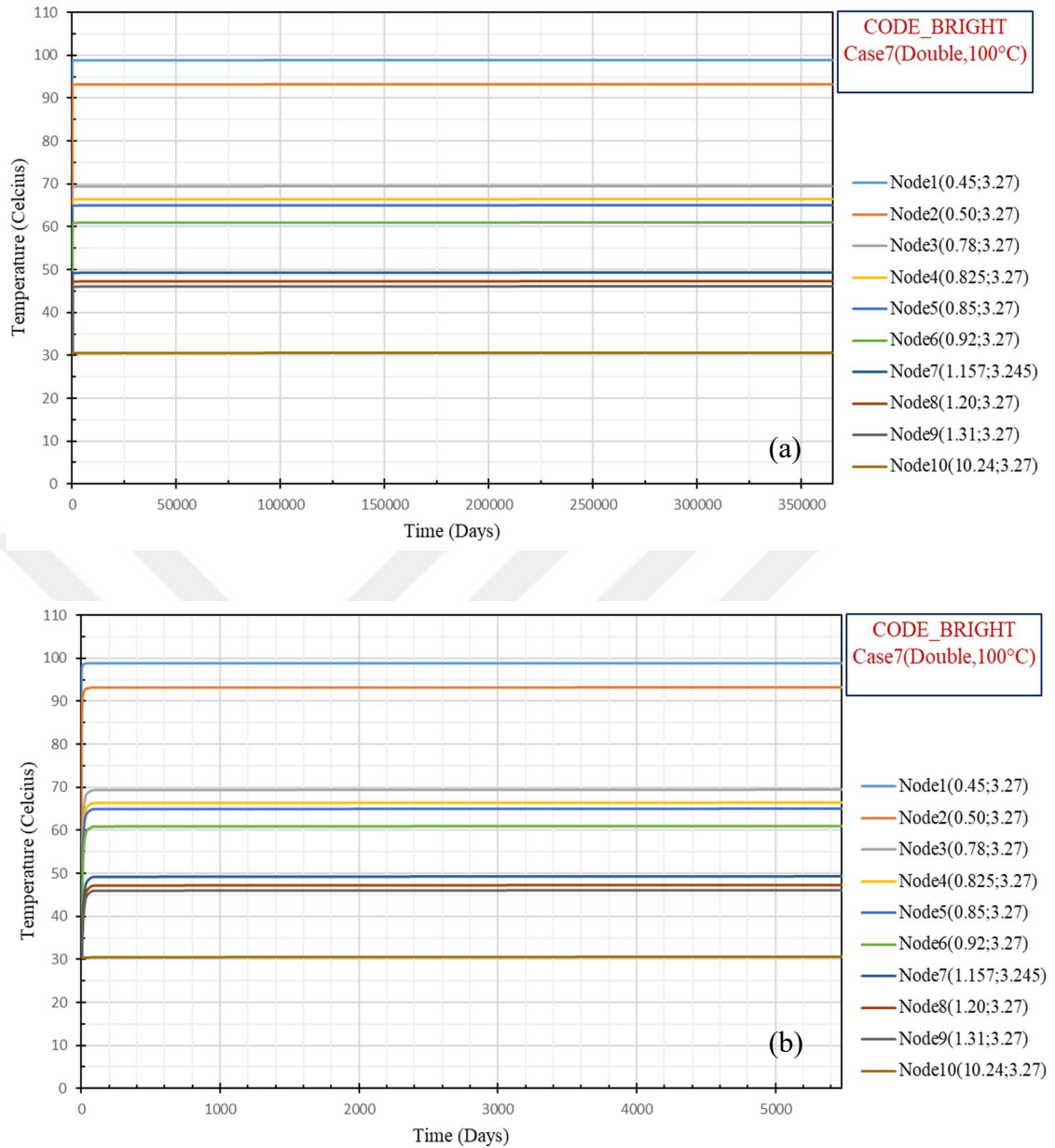


Figure 3.23 The graph of temperature at different positions from canister has double layer buffer by using 100°C conditions analysis by CODE_BRIGHT: (a)Time up to 1000 years, (b)Time up to 15 years

As a result of the model Case7, where the canister surface was kept at 100°C, it can be seen from Figure 3.23 (a) that the temperature of Node2, which was 0.05 m away from the canister surface, was approximately 93°C. The temperatures of Node3, which was at the intersection of two layers and 0.33 m away from the canister surface, and Node4, which was 0.375 m away from the canister surface, were found to be 69°C and 66°C (Figure 3.24(a)). The temperatures of Node5, Node6, Node7, which were inside

the second buffer layer, were 65°C, 61°C and 49°C after 1000 years, respectively. The temperature at Node8, which was at the buffer–host rock intersection was calculated to be 47°C. The temperatures of two nodes inside the rock, Node9, 0.86 m away from the canister surface and Node10, 9.79 m away from the canister surface, were found to be 46°C and 31°C after the 1000-year analysis time. It can be seen from Figure 3.23 (b) that temperature values at all nodes reached a steady state after approximately 40 days.

The thermal analysis results for the Case8 model designed as a double layer, heat flux was used as the flow BC, obtained over 1000 years and 15 years are shown in Figure 3.24 (a) and (b).

It can be seen from Figure 3.24 (a) that the temperature of Node1 on the canister surface reached a maximum value (82°C) and decreased to 36°C after 1000 years. The temperature at Node2, which was 0.05 m away from the canister surface, increased to 78°C and decreased to about 35°C after 1000 years. Temperatures for Node 3, which was at the intersection of two layers and 0.33 m away from the canister surface, and Node4, which was 0.375 m away from the canister surface were found to be 59°C and 57°C, respectively. Temperatures of Node5, Node6 and Node7, where the 15T-68S-17B mixture was used as the second buffer layer, were calculated to be 56°C, 53°C and 44°C, respectively. The maximum temperature was found to be 43°C for Node8, which was at the intersection of 15T-68S-17B and the granite (host rock). Temperatures of Node9 and Node10 inside the rock, whose coordinates were [1.31;3.27], were 42°C and 31°C, respectively.

It can be seen from Figure 3.24 (a) and (b) that temperatures at all nodes reached the maximum within 40 days and decreased well below 40°C after 1000 years.

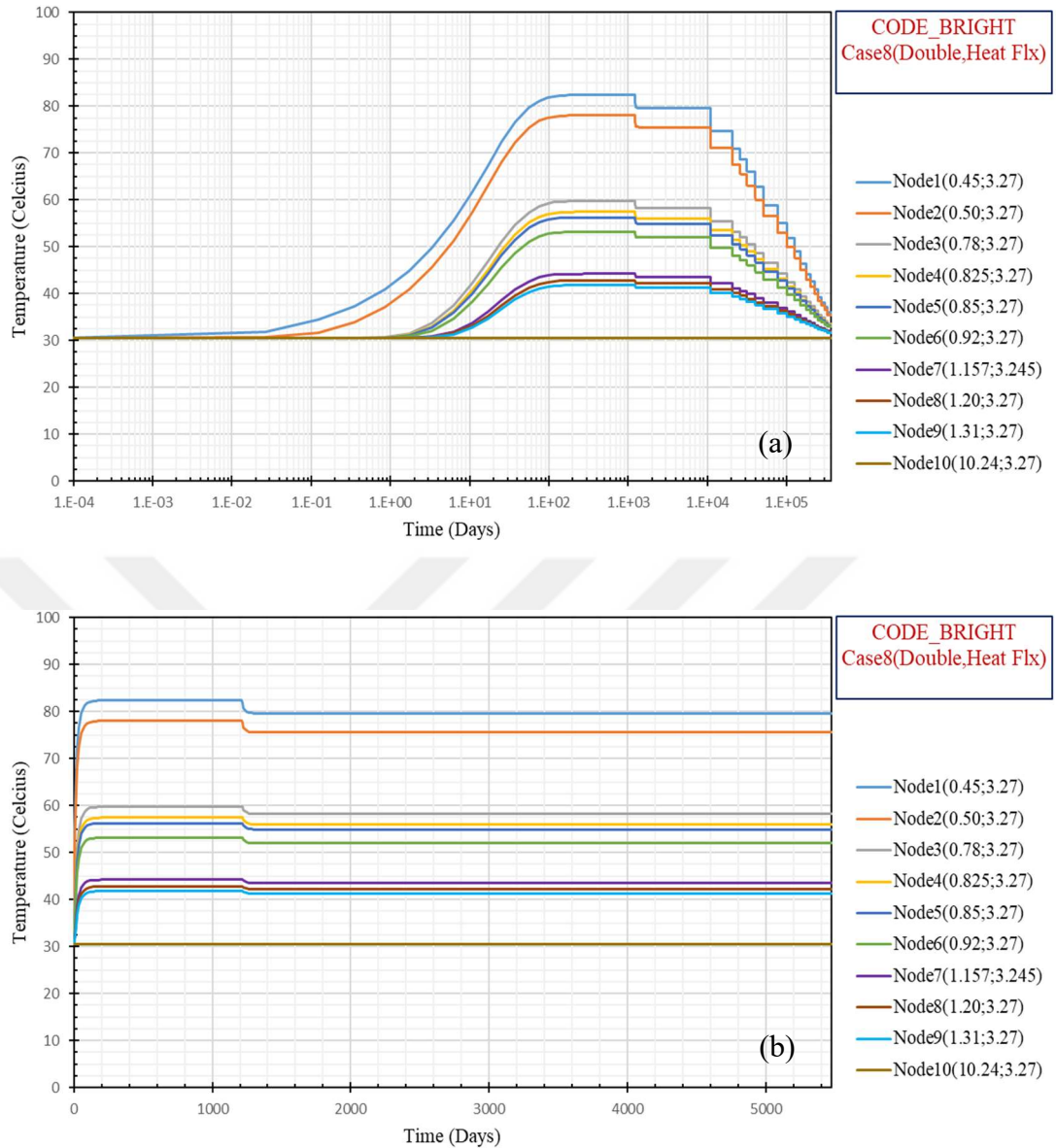


Figure 3.24 The graph of temperature at different positions from canister has double layer buffer by using heat conditions analysis by CODE_BRIGHT: (a)Time up to 1000 years, (b)Time up to 15 years

3.5 Comparison of ANSYS, GID and PEBS-CIMNE Analysis Results

In this section, the results obtained by ANSYS 2019 R1 and CODE_BRIGHT software were compared with those calculated in the PEBS project. The results given in the PEBS report could not be found in a tabular form, thus values were read from the graphs.

Table 3.17 (a) and (b) shows the analysis results of the model – designed as a single-layer buffer using the 15T-68S-17B mixture – performed under constant canister surface temperature and heat flux flow conditions, as well as the THO (thermo-osmosis) analysis results of the model using FEBEX bentonite as a buffer performed by the CIMNE group within the scope of the PEBS project.

Table 3.17 The results of single layer buffer analysis by ANSYS 2019 R1, CODE_BRIGHT and PEBS-CIMNE: (a) Constant canister temperature (100°C), (b) Heat flux from canister surface

	ANSYS 2019 R1 Case1 (Single ; 100°C)	CODE_BRIGHT Case5 (Single ; 100°C)	EURATOM-PEBS CIMNE (THO)(100°C)
Node1 [0.450;3.27]	100	100	100
Node2 [0.500;3.27]	93	93	96
Node3 [0.820;3.27]	64	67	78
Node4 [1.200;3.27]	47	48	60
Node5 [10.24;3.27]	31	31	35

(a)

	ANSYS 2019 R1 Case2 (Single ; Heat Flux)	CODE_BRIGHT Case6 (Single ; Heat Flux)	EURATOM-PEBS CIMNE (THO)(Heat Flux)
Node1 [0.450;3.27]	79	81	97
Node2 [0.500;3.27]	75	77	90
Node3 [0.820;3.27]	55	57	65
Node4 [1.200;3.27]	43	43	52
Node5 [10.24;3.27]	31	31	31

(b)

The distances of the nodes from canister surface are shown in Figure 3.25. It can be seen from Table 3.17 (a) and (b) that ANSYS 2019 R1 and CODE_BRIGHT software had very similar results to each other. The results were assumed to be the same because the same model geometry, mesh and boundary condition and mixtures were used in the design; however, the reason for a 2°C temperature difference was due to the difference between the thermal conductivity values defined in the programs. In the ANSYS 2019 R1 program, the λ value was defined as λ_{wet} at 25°C and as λ_{dry} at 100°C with a linear equation decreasing with increasing temperature, and the program calculated the λ value used for each temperature change by means of linear

interpolation. However, because this was not possible in the CODE_BRIGHT software, λ was calculated by averaging λ_{dry} and λ_{wet} values.

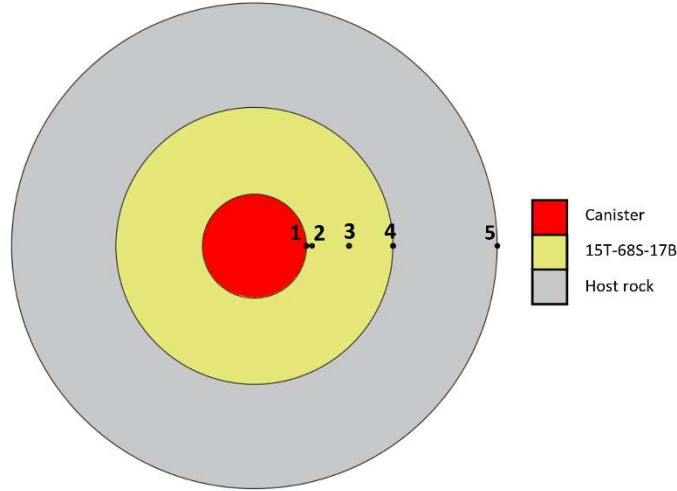


Figure 3.25 The distances of the node points from canister surface

In the model analyzed by the CIMNE group using bentonite as a buffer, the temperature of the point in the buffer in contact with the canister surface increased to around 97°C – due to heat energy generated by spent fuel – and decreased with time. From among the boron-added sand–bentonite mixtures with calculated thermal conductivity values, the single layer system where 15T-68S-17B was used as a buffer had a temperature at the buffer point in contact with the canister surface that reached 80°C. As a result, the use of the 15T-68S-17B mixture achieved a 17°C temperature decrease on the canister surface compared to bentonite.

Because of the absorptive capability of colemanite to make neutron particles stable, the double-layer buffer design was tested and the results of analyses using ANSYS 2019 R1 and CODE_BRIGHT software are shown in Table 3.16 (a) and (b). Because only a single-layer system was analyzed within the scope of the PEBS project, a comparison with these results was not possible.

It can be seen in Table 3.18 (a) and (b) that the temperature difference in the buffer between the analysis results for ANSYS and CODE_BRIGHT software was

approximately 3°C under constant canister surface temperature conditions and about 2°C under heat flux BCs. The reason for this difference was explained in previous paragraphs. The maximum temperature of the point on the canister surface in the single-layer model using 15T-68S-17B material as a buffer was less than that in the double-layer buffer model by approximately 1°C under heat flux BCs. This is due to the fact that the thermal conductivity value of the material with colemanite is slightly less than that of the material with tincal.

Table 3.18 The results of double layer buffer analysis using ANSYS and CODE_BRIGHT: (a) Constant canister temperature (100°C), (b) Heat flux from canister surface

	ANSYS 2019 R1	CODE_BRIGHT
	Case3 (Double ; 100°C)	Case7 (Double ; 100°C)
Node1 [0.450;3.27]	100	100
Node2 [0.500;3.27]	93	93
Node3 [0.780;3.27]	66	69
Node4 [0.825;3.27]	63	66
Node5 [0.850;3.27]	62	65
Node6 [0.920;3.27]	58	61
Node7 [1.157;3.27]	48	49
Node8 [1.200;3.27]	47	48
Node9 [1.310;3.27]	46	46
Node10 [10.24;3.27]	31	31

(a)

	ANSYS 2019 R1	CODE_BRIGHT
	Case4 (Double ; Heat Flux)	Case8 (Double ; Heat Flux)
Node1 [0.450;3.27]	80	82
Node2 [0.500;3.27]	76	78
Node3 [0.780;3.27]	57	59
Node4 [0.825;3.27]	55	57
Node5 [0.850;3.27]	54	56
Node6 [0.920;3.27]	51	53
Node7 [1.157;3.27]	44	44
Node8 [1.200;3.27]	43	43
Node9 [1.310;3.27]	42	42
Node10 [10.24;3.27]	31	31

(b)

The temperature of the node inside the rock, which was approximately 9.79 m away from the canister surface, was found to be 31°C after 1000 years for all conditions. Considering that the distance between the centers of canisters inside next two shafts is 35 m, the final temperature of a node 9.79 m away from a canister surface is very close to the initial temperature value, which indicates that the distance between the two shafts is adequate, and there will not be any thermal horizontal interference between canisters. This important result is presented in Figure 3.26.

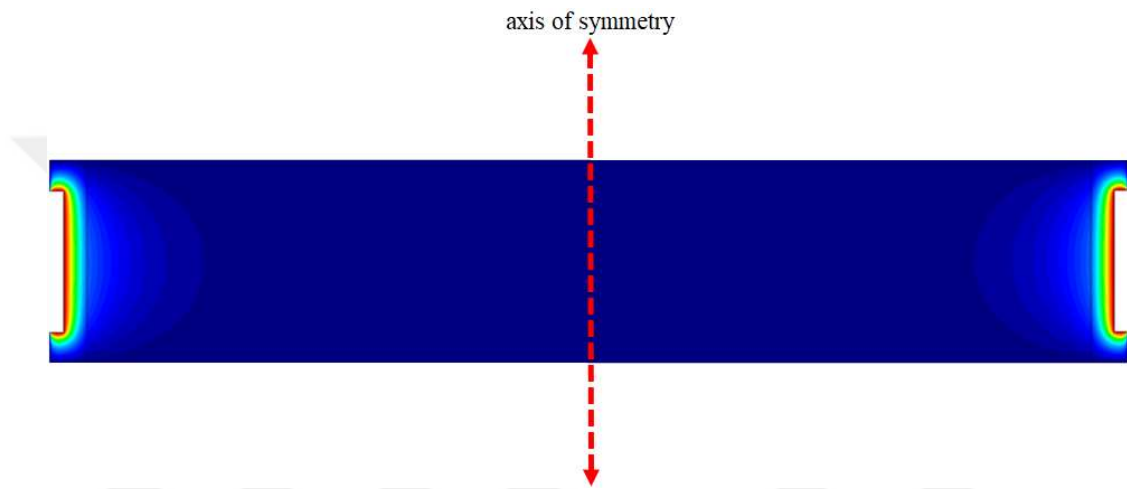


Figure 3.26 Thermal analysis of two canisters in the consecutive disposal drifts using CODE_BRIGHT

CHAPTER FOUR

CONCLUSIONS AND RECOMENDATIONS

4.1 Conclusions

In this study, the thermal conductivity values of boron-added sand–bentonite mixtures were determined, and by using these values, buffers surrounding the canisters in horizontally modeled shafts in nuclear waste repositories were thermally designed and analysed. The results obtained throughout this study are summarized below:

- There is an optimum fine content range that affects thermal conductivity behavior in sand–bentonite mixtures. It is considered that this fine grain size, i.e. the bentonite ratio, is between 15% to 25%.
- Among boron-added sand–bentonite mixtures, the lowest and highest thermal conductivity values were obtained in 5T-76S-19B and 15T-68S-17B mixtures with the addition of tincal.
- When 5% boron is added into the sand–bentonite mixtures, thermal conductivity values decrease; however, with added boron above 5%, thermal conductivity values increase.
- The lowest thermal conductivity value is obtained when added boron is $\leq 5\%$, and using boron greater than 5% increases thermal conductivity.
- One of the most important factors affecting the thermal conductivity coefficient of porous mixtures is the fine grain content of the mixture.
- The thermal conductivity coefficient (λ), which is included in the general heat equation, determines the maximum temperature value that can form in the material due to heat transfer mechanisms. The volumetric heat capacity of a material ($\rho c_{p,f}$) determines the temperature that the material will reach after a

certain time – for short-term analyses – and the time to reach that temperature. The heat diffusion coefficient (α) affects the transfer rate of heat stored by the material itself and the heat transferred to it.

- It is considered that boron-added sand–bentonite mixtures can be used rather than using bentonite alone to serve as a buffer in disposing HLW.
- It is also considered that because sand–bentonite mixtures with colemanite have the capability to capture radioactive neutron particles, using them as buffer material will be more beneficial compared to other boron-added mixtures.
- In the buffer designed with a double layer, a temperature increase that does not exceed the upper limit (100°C) is observed (max 80°C). Moreover, about a 17°C maximum temperature decrease was observed on the canister surface when compared with the use of bentonite alone.

4.2 Recommendations for Future Research

In this thesis, the thermal conductivity of boron added sand-bentonite mixtures determined. Instead of bentonite material used as a buffer around canister where waste is stored in nuclear waste repositories, boron added sand-bentonite mixtures were used in this thesis, single and double layer structures were designed separately and analyzed with the help of two different computer program using finite element method. According to results of this study, it was seen that the boron minerals can be used in the buffer materials in order to decrease the temperature at the canister surface and inside the buffer. Based on the thesis, the following recommendations for future research are suggested:

- The thermal conductivity of soils change depending on temperature. For that reason, the thermal conductivity and specific heat of sand-bentonite mixtures should be determined under different temperature conditions.

- Further research is needed in terms of thermo-hydro-mechanical (THM), radiological and chemical analysis.
- The canister, buffer and host rock system can be modeled in laboratory scale and heat, water transport can be investigated under THM conditions.
- The boron nucleus captures neutrons emerging from nuclear waste areas to form more stable compounds. The radiation prevention capacity of colemanite added sand-bentonite mixtures should be investigated experimentally.



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APPENDICES

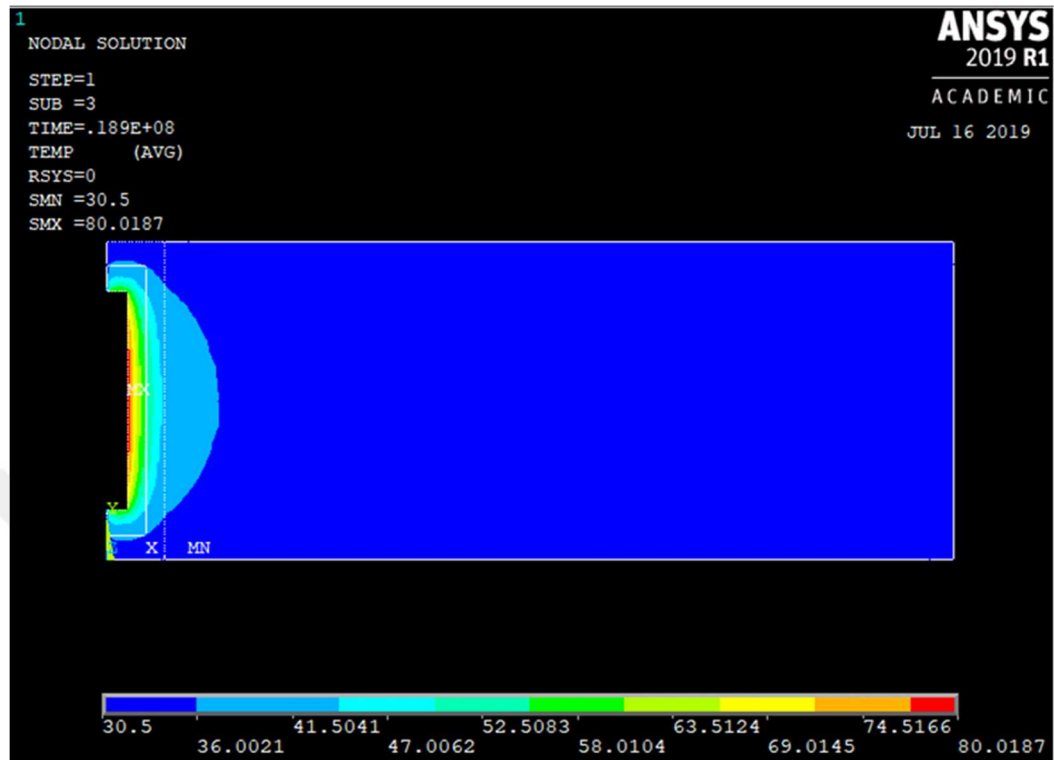


Figure A.1. Contours of double layer buffer (ANSYS)

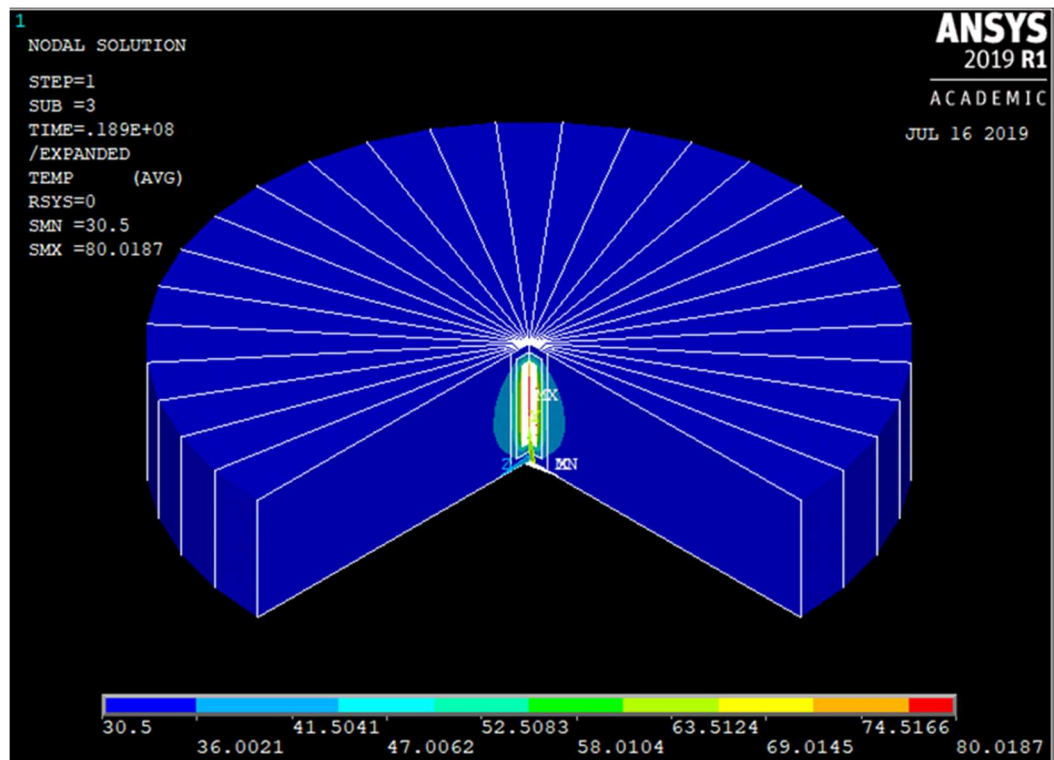


Figure A.2. $\frac{3}{4}$ expansion of model (ANSYS)

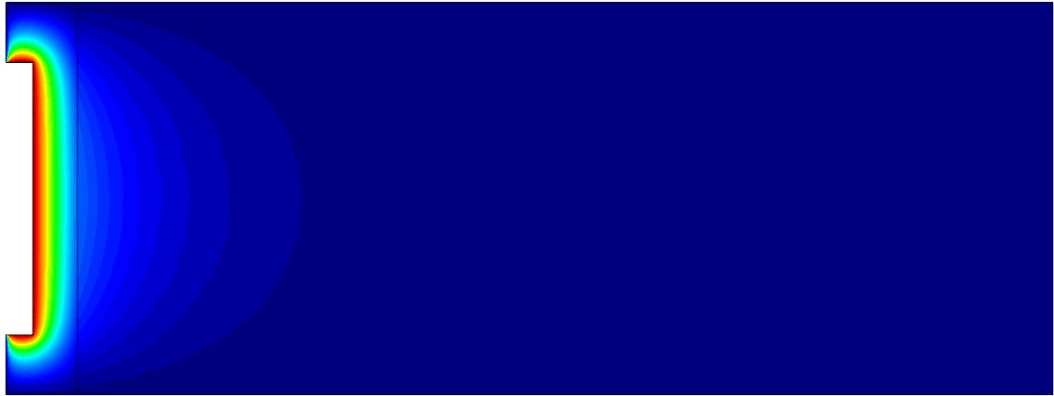


Figure A.3. Contours of single layer (CODE_BRIGHT)



Figure A.4. Vectors of i heat conducti (CODE_BRIGHT)

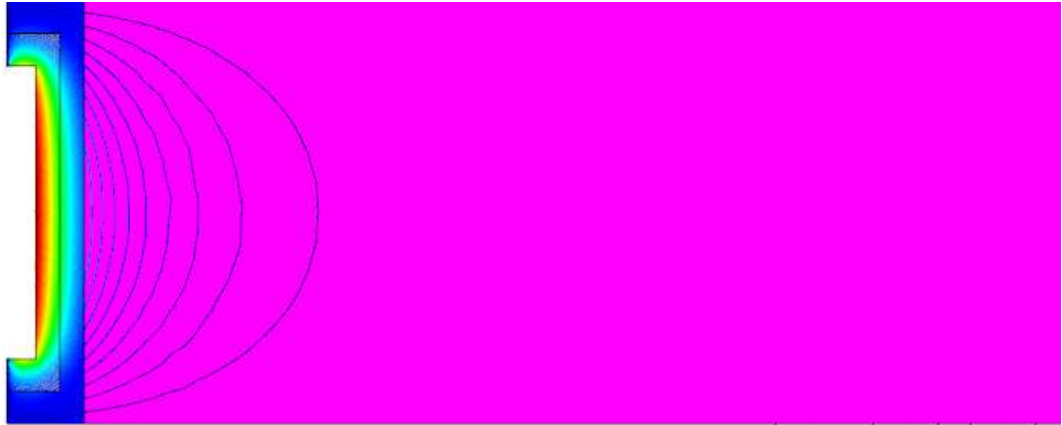


Figure A.5. Contours of double layer (CODE_BRIGHT)



Figure A.6. Vectors of κ heat conductivity (CODE_BRIGHT)