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THE MODELING METHOD OF DIFFUSION OF RADIO ACTIVATED MATERIALS IN CLAY WASTE DISPOSALS

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ABSTRACT

These days the need for more electricity power and also arrival of new technologies which are related to the nuclear energy, force us to build new nuclear plants. Nuclear power is the only large-scale energy-producing technology which takes full responsibility for all its wastes .The amount of radioactive wastes is very small relative to wastes produced by fossil fuel electricity generation. However used nuclear fuel may be treated as a resource or simply as a waste.Nuclear wastes are particularly hazardous and hard to manage relative to other toxic industrial wastes. Here in this article we are going to evaluate three methods to model the diffusion of the burred waste from waste source to the ground surface. For this purpose three soft wares such as *ABAQUS, Matlabcoding* and *Geostudio* (seep/w &Ctran/w) has been used. At the end, the results will be compared with each other and the final results will be presented. It is noteworthy that using these models can help the headmasters to control the nuclear waste more safely and prevent from dangerous effects of nuclear energy.

Keywords: Nuclear power, radioactive waste, diffusion model, Abacus, Matlab, Geostudio

1. INTRODUCTION

Almost all parts of a nuclear fuel cycle can produce radioactive waste (rad-waste) and the cost of managing and disposing of this waste is part of the electricity cost, it means that all the cost should be paid by the electricity consumers. For each stage of the fuel cycle there are useful technologies to dispose of the radioactive wastes safely. Most of these technologies can be applied for low- and intermediate-level wastes. For high-level wastes some countries use special methods to await the accumulation of it and also to warrant building geological repositories. Unlike other industrial wastes, the risk level all nuclear waste - its radioactivity - decreases with time. It is clear that each radionuclide waste has a half-life which is the time taken for half of its atoms to decay. Radionuclides with long half-lives tend to emit alpha and beta that makes their handling easier but those with short half-lives tend to emit the more penetrating and dangerous gamma rays. It is clear that all of radioactive wastes will decay into non-radioactive elements. It is a rule that the more radioactive an isotope is, the faster it decays. The final goal in managing and disposing of radioactive waste is to protect people and the environment. This means that isolating or diluting the waste can decrease concentration of any harmful radionuclide. To achieve this, practically all wastes need clearly deep and permanent burial. For nuclear power generation this protection should be more precise. All toxic wastes include radioactive waste need to be disposed safely. In countries with nuclear power, such as Iran, radioactive wastes comprise about 1% of total industrial toxic wastes (that is considered ad hazardous waste).

1.2. Types of radioactive wastes

1.2.1. Very Low level waste

Very low level waste (VLLW) include radioactive materials with a risk level which is not considered as a harmful agent to people or their environment. These wastes consist mainly of demolished material (such as concrete, plaster, bricks, metal, valves, piping etc.) which are produced during rehabilitation or dismantling operations of nuclear industrial sites.

1.2.2. Low-level waste

Low-level waste (LLW) is can produced by hospitals, industry, and the nuclear fuel cycle. It includes paper, rags, tools, clothing, and filters which contain small amounts short-lived radioactive material. It does not require any special shielding during handling and transport and to dispose of this kind of waste it is better to use shallow land burial.

To reduce its volume, it is recommended to compact or incinerate it before disposal. This type of waste comprises about 90% of the volume of all the nuclear waste but only 1% of the radioactivity of all radioactive waste.

1.2.3. Intermediate-level waste

Intermediate-level waste (ILW) includes higher amounts of radioactivity and some of these waste requires shielding. It includes resins, chemical sludge and metal fuel cladding and also contaminated materials from reactor decommissioning. Smaller items and any non-solids may be solidified in concrete or bitumen for disposal. This type of waste includes about 7% of the volume of all radioactive wastes and has 4% of the radioactivity of all radioactive waste. In another words, its radioactive decay can generate heat of less than about 2 kW/m^3 so its heat doesn't need to be considered in design of storage or disposal facilities.

1.2.4. High-level waste

High-level waste (HLW) can produce from 'burning' of uranium fuel in a nuclear reactor. HLW includes the fission products and transuranic elements generated by the reactor core. It is highly radioactive and also dangerous because of heat emitted due to decay process so requires cooling and shielding. Its thermal power is about 2 kW/m^3 and can be considered as the 'ash' from 'burning' uranium. HLW is considered as over 95% of the total radioactivity generated in the process of electricity generation. HLW has both long-lived and short-lived components, their risk level depends on the length of time it will take for the radioactivity of particular radionuclides to decrease to safe levels and after that it will be harmless to surrounding environment. Separating the generally short-lived fission products can be so important in management and disposal of HLW.

1.2. Mining and milling

Traditional uranium mining method generates fine sandy tailings, which contain virtually all the naturally occurring radioactive elements which can naturally be found in uranium ore. These materials are collected in engineered tailings dams and finally covered with a layer of clay and cemented rock to prevent the leakage of radon gas and ensure long-term stability of the disposal system. In the short term, the tailings material is often covered with water. After a few months, the tailings material contains about 75% of the radioactivity of the original ore but generally these are not classified as radioactive wastes.

1.3. Conversion, enrichment, fuel fabrication

Uranium oxide concentrate which is considered as 'yellowcake' ($U3O8$), is not significantly radioactive. After refining, it would convert to uranium hexafluoride gas ($UF6$). As a gas, by the use of enrichment process the U-235 content increase from 0.7% to about 3.5%. It is then turned into a hard ceramic oxide ($UO2$) for assembly as reactor fuel elements.The main byproduct of enrichment is depleted uranium (DU), which is the U-238 isotope, and also is stored as UF6 or U3O8 .By this moment about 1.2 million tons of DU is now stored all over the world.

1.4. Managing high-level wastes (HLW)

Used fuel can be converted into high-level wastes (HLW) which may include used fuel itself in fuel rods, or the separated waste generated from reprocessing of this. In either case, the amount is modest – as noted above, a typical reactor generates about 27 tons of used fuel which may be reduced to 3 m^3 per year of vitrified waste. Both of these materials can be effectively and economically isolated, and also can be handled and stored safely since nuclear power began. As noted before, the HLW produce a considerable amount of heat and requires cooling. It is vitrified into borosilicate (Pyrex) glass, encapsulated into heavy stainless steel cylinders about 1.3 meters high and at the end will be stored for deep underground disposal. This material has no future application and is unequivocally waste. The hulls and end-fittings of the reprocessed fuel assemblies should be compacted, to reduce volume, and usually incorporated into cement prior to disposal as ILW. If used reactor fuel is not reprocessed, it will contain all the highly radioactive isotopes that are considered as dangerous material which is treated as HLW for direct disposal. This type of waste generates a lot of heat and again requires cooling. However, since it largely consists of uranium (with a little plutonium), it represents a potentially valuable resource and there is an increasing reluctance to dispose of it irretrievably. It is notable that after 40-50 years the heat and radioactivity level will fall to one thousandth of the level at removal time. This provides an important technical incentive to delay further action with HLW until the radioactivity has reduced to about 0.1% of its original level.

1.5. High Level Waste Decay

A current important question is whether wastes should be emplaced. There are possible reasons for keeping such options open – in general condition, it is possible that future generations might consider the buried waste to be a valuable resource of energy. On the other hand, permanent closure might increase long-term security and also safety of the facility. It is clear that after being buried for about 1,000 years most of the radioactivity will have decayed. Then remaining the amount of radioactivity would be similar to naturally-occurring uranium ore level, though it would be more concentrated.

1.6. DisposalOptions

1.6.1. Near-surface disposal

1.6.1.1. Near-surface disposal facilities at ground level

These facilities are on or below the surface and the protective covering layer has a few meters thick and also waste containers are placed in constructed vaults that are backfilled. Finally the mentioned structure will be covered and capped with an impermeable membrane. These facilities may incorporate some type of drainage and also a gas venting system.

1.6.1.2. Near-surface disposal facilities in caverns below ground level

Unlike near-surface disposal systems in which the excavations are conducted from the surface, shallow disposal requires underground excavation of caverns where the facility will locate at depth of several tens of meters below the Earth's surface and accessed through a drift.

These facilities can be affected by long-term climate changes (such as glaciation) and this effect must be considered in safety design since such changes could cause disruption of these facilities. Therefor this type of facility can typically be used for LLW and ILW with a radionuclide content of short half-life (up to about.30.years).

1.6.2. Deep geological disposal

The long time intervals on which some of the waste remains radioactive led to the idea of using deep geological disposal in underground repositories which are located in stable geological formations. Isolation process can be provided by a combination of engineered and natural barriers such as rock, salt and clay. This system is often defined as a multi-barrier term, which includes the waste packaging, the engineered repository and also the geology which all providing barriers to prevent the radionuclides to leak.

1.6.2.1. Mined repositories

The main concept of this section depends on repository comprising mined tunnels or caverns into which packaged radioactive waste would be placed. In some cases (e.g. wet rock) material such as cement or clay (usually bentonite) can be used to create a cover layer for the waste to provide another barrier which its process is shown in figure 2 (called buffer and/or backfill). The choice of waste container or buffer/backfill materials and its design depends on the type of radioactive waste and the nature of the host rock. It noteworthy that" deep geological disposal" is the best option for waste management of long-lived radioactive waste in several countries, including Argentina, Australia, Belgium, Czech Republic, Finland, Japan, Netherlands, Republic of Korea, Russia, Spain, Sweden, Switzerland and USA. From the studies of the deposits of native (pure) copper in the world it has been proven that the copper which is used in the final disposal container can remain unchanged inside the host rock for extremely long periods, if the geochemical conditions are appropriate (reducing groundwater). The findings of ancient copper tools, many thousands of years old, also states the long-term corrosion resistance of copper, making it a vulnerable container material for long-term radioactive waste storage.

1.6.2.2. Deep boreholes

As well as mined repositories, deep borehole disposal method for high-level radioactive waste has been considered as an alternative option for geological isolation. This method includes drilling a boreholes into crystalline basement rock to a depth of about 5000 meters, emplacing waste canisters containing used nuclear fuel or vitrified radioactive waste from reprocessing in the lower 2000 meters of the borehole, and sealing the upper 3000 meters of the borehole with materials such as bentonite, concrete or asphalt. The disposal zone of a single borehole can contain 400 steel canisters each 5 meters long and one-third to half a meter diameter. These might be emplaced in strings of 40 canisters. The waste containers can separated from each other by a thin layer of bentonite or cement. Boreholes can be readily drilled host rocks like crystalline and sedimentary. This capability significantly expands the range of locations that can be considered for using the disposal of radioactive waste.

2. MATERIALS AND METHODS

2.1. History of the research

Here in this section we are going to introduce some use full studies that have been conducted in the field of radioactive waste diffusion and methods of its disposal. One of the most attractive discussions in this field is *"Uranium Diffusion in Soils and Rocks"*which has done by Stephanie M. Moore. For readers who want to understand more about radioactive diffusion we recommend *"Diffusion of Radionuclides in Concrete and Soil"* which has studied by group of researchers such as Shas V. Mattigod, Dawn M. Wellman, Chase C. Bovaird, Kent E. Parker, Kurtis P. Recknagle, Libby Clayton and Marc I. Wood. Furthermore *"Diffusion and Leaching*

Behavior of Radionuclides in Category 3 Waste Encasement Concert and Soil Fill Material" can be considered as a comprehensive source to whom he or she wants to know more about radioactive waste disposal.

2.2. Site introduction

Here in this article we try to evaluate a site containing a radioactive waste that is buried at the depth of 50m from the ground surface and its height is equal to 20 meters. By using two different analysis the waste diffusion from the depth to the surface will be modeled and also the seismic behavior of the waste bulk will be evaluated. For this purpose we will use three well-known software and then the results will be compared. Figures of 4 and 5 show the geometry of this site for two conditions (assuming the soil is as one layer profile and 3 layer profile).

2.3. Waste Diffusion Model

The governing equation for transient radioactive waste diffusion accounting for trapping and hydrostatic drift are given by

Equation 1

$$\frac{D_L}{D_{eff}}\frac{\partial C_L}{\partial_t} - D_L\nabla^2 C_L + \nabla.\left(\frac{D_L C_L V_H}{3RT}\nabla\sigma_{kk}\right) + \alpha\theta_T\frac{dN_T}{d\varepsilon_p}\frac{\partial\varepsilon_P}{\partial t} = 0$$

2Equation

$$D_{eff} = \frac{D_L}{\left[\frac{C_L + C_T(1-\theta_T)}{C_L}\right]}$$

Where $\partial/\partial t$ is the time derivative. In Eq. (1), D_L is the waste diffusion constant through NILS; D_{eff} is an effective diffusion constant that varies point wise; C_T is the waste concentration per unit volume in trapping sites; C_L is the waste concentration per unit volume in normal interstitial lattice sites (NILS); θ_T denotes the occupancy of the trapping sites; N_T denotes the trap density which is a function of the local effective plastic strain ε_p i.e., $N_T = N_T(\varepsilon_p)$, and is measured in number of traps per unit volume. To incorporate the waste induced lattice deformation, the deformation rate D_{ij} should be calculated from

Equation3

$$D_{ij} = D_{ij}^e + D_{ij}^p + D_{ij}^t$$

With$D_{ij}^e, D_{ij}^p, D_{ij}^t$denote the elastic part, the plastic part and the part due to lattice straining by the solute waste. The waste induced deformation rate $D_{ij}^t$is purely dilatational and, in the context of the large strain formulation, is given by Asian Pacific Conference for Materials and Mechanics 2009 at Yokohama, Japan, November 13-16

Equation4

$$D_{ij}^{t} = \frac{d}{dt}\left\{\ln\left[1 + \frac{(C - C_0)\Delta\upsilon}{3\Omega}\right]\right\}$$

Where C is total waste concentration (in NILS and trapping sites) measured in waste atoms per solvent atom; C_o is the initial waste concentration in the absence of any straining;$\Delta\upsilon$ is the volume change per atom of waste introduced into solution that is directly related to the partial molar volume of waste $V_H = \Delta\upsilon\ N_A$ in solution; and Ω is the mean atomic volume of the host metal atom. To model the diffusion of radioactive waste, in this article we will use the ABAQUS software (seismic and non-seismic conditions), MATLAB coding (seismic mode) and Geostudio (Seep/w &Ctran/w) for non-seismic mode.

3. RESULTS AND DISCUSSION

3.1. Finite Element Implementation to ABAQUS

To implement constitutive equations for waste diffusion, two user subroutines within ABAQUS are developed. The first one is UMATHT to define a material's thermal behavior for the heat transfer analysis (in this paper waste diffusion analysis), and the second one UMAT to define a material's mechanical behavior to incorporate deformation rate induced due to lattice straining by the solute waste.

ABAQUS provides the built-in program for the heat transfer analysis. An interesting point is that the governing equation for the heat transfer analysis is similar to that for transient waste diffusion given in Eq. (1). For modeling the waste distribution from the depth to the ground surface we will use ABAQUS's thermal distribution model to do this we have to take the thermal coefficient factor equal by diffusion coefficient factor. The reason for taking the same value is that the equations that use for thermal distribution are similar to diffusion model. Figure 5 to 9 show the waste diffusion model for non-seismic mode. And also to evaluate the diffusion model in seismic conditions; we applied the PGA factors of Loma earthquake acceleration charts, to consider this PGA values we assume the ratio of 1.5 to the right side of the model. This ratio is derived from MATLAB coding operation. Figures of 6-13 show the seismic model of waste distribution.

3.2. MATLAB coding

It is proved that the Ratcliff diffusion model is a useful tool in reaction time analysis.

However, its application has been limited by difficulty in estimation of the parameters. Here we are going to present a software tool, the Diffusion Model Analysis Toolbox (DMAT) which is intended to make the Ratcliff diffusion model for reaction time and accuracy data more accessible. The tool takes the form of a MATLAB tool box. Using this program does not require a background not only in mathematics, but also any advanced programming experience (but familiarity with MATLAB is useful). DMAT features both a graphical user interface (GUI) and a command interface (CI). To start the GUI, simply type "dmatgui" in the MATLAB command window. Using the GUI should be largely self-evident if the commands for the CI are known.

The first step to model a diffusion model in MATLAB software is to get the PGA factor. For this purpose we downloaded the acceleration, displacement and velocity charts of Loma earthquake from the http://ngawest2.berkely.edu site .The acceleration charts are depend upon some parameters such as fault properties, magnitude of the earth quake and also type of the soil in which the waves was dispersed.

By using PGAfactor we found a ratio which has been used in pervious section, and again in this section we will directly use it in diffusion equation. Increase in the velocity factors of diffusion make the velocity distribution vector to be non-symmetrically which has shown in figure 15. By using the velocity vectors we can now model the diffusion of waste in 2D mode for different time sections. Figures of 14 to 18 show the diffusion process.

3.3. Advection/dispersion analysis using Geo studio

It is noteworthy that CTRAN/W is always used in combination with SEEP/W or VADOSE/W, finite element programs that are most important part of the GeoStudio product line. The first step is to model the flow regime. To start this lesson, we are going to conduct a contaminant transport simulation for the following profile. A pit containing a contaminant fluid with a relative concentration of 12 kg/m3.The CTRAN/W analysis will be an advection/dispersion analysis, which will model the concentration of the contaminant plume as it advances through the profile with time. Contaminant/radioactive waste diffusion is considered inconsequential and is ignored in this particular analysis. The geometry is considered project specific, but you can change boundary conditions, material properties, and even different types of analyses. CTRAN/W will use the existing

SEEP/W results, so this means the SEEP/W analysis is the parent of the CTRAN/W analysis. The time that we are going to model is approximately 10 years or 3650 days.Let us analyze 120 time steps, with 30-day increments, the time steps have been flagged to save results for every 3th time. To define the contaminant transport properties for the soil, we need to go under KEYIN, Materials. Boundary conditions will at first created and then will be assigned to the geometry using DRAW. Boundary conditions in this example are continuous injection of contaminant which is assumed to exist along the surface waste bulk and the relative concentration along these nodes will be set to 10. The nodes that exist on the ground surface will be defined as a free exit boundary, which allows both dispersive and advective fluxes to cross. Figures of 19 to 21 show the mentioned process.

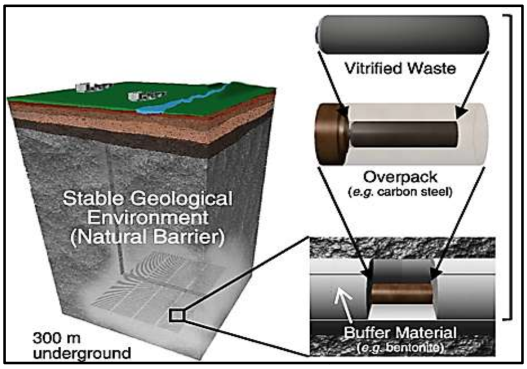

Fig. 1 Disposal process of radioactive waste in wet rocks [1]

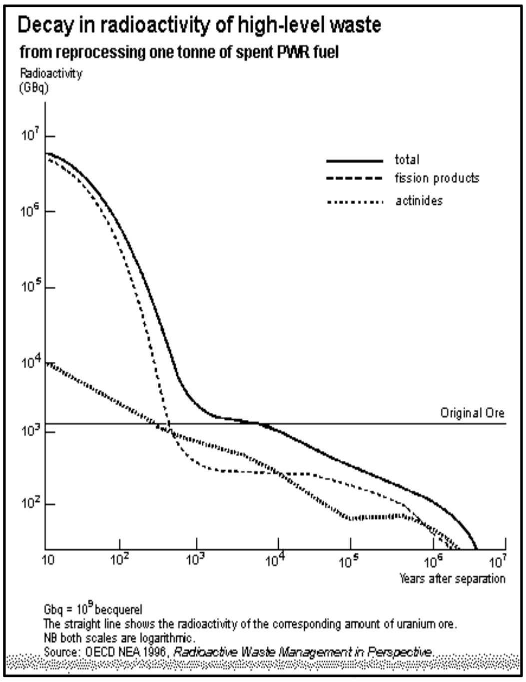

Fig. 2 Decay in radioactivity of high-level waste from one ton of spent PWR fuel [1]

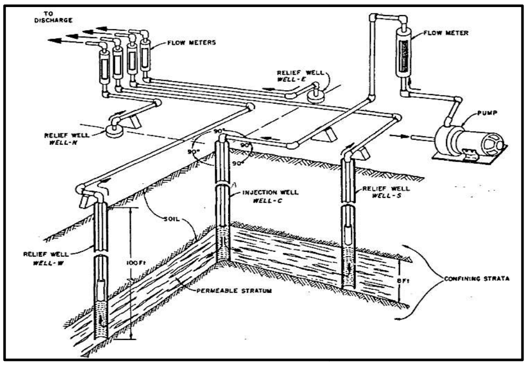

Fig. 3 Near-surface disposal facilities [1]

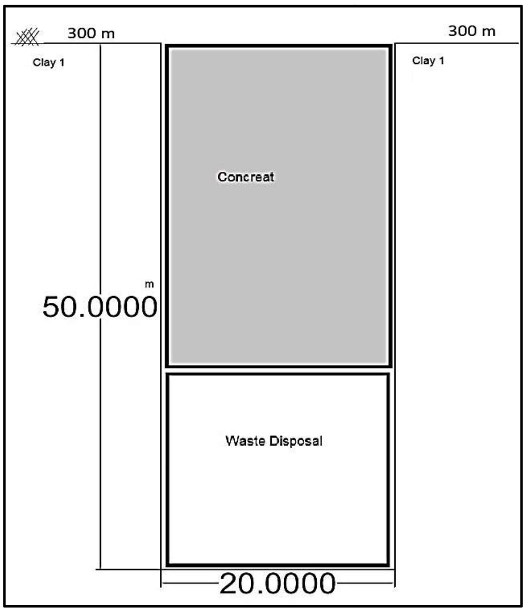

Fig. 4 Soil profile of the study site by assuming the soil as one layer

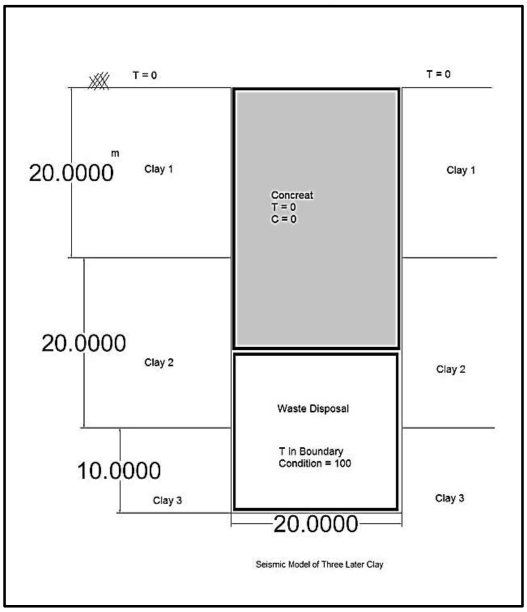

Fig. 5 Soil profile of the study site by assuming the soil as 3 layers

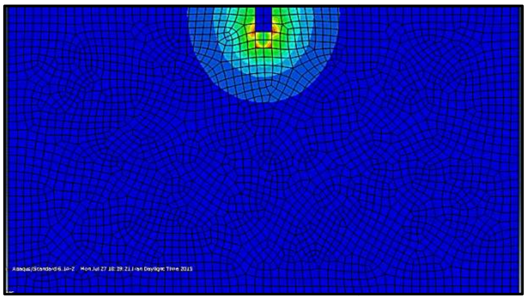

Fig. 6 Diffusion model conducted with ABAQUS for non-seismic mode, one layer profile and initial condition

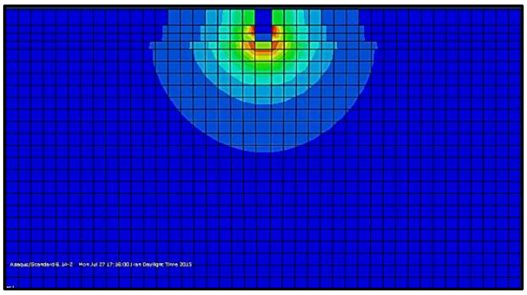

Fig. 7 Diffusion model conducted with ABAQUS for non-seismic mode, 3 layer profile and initial condition

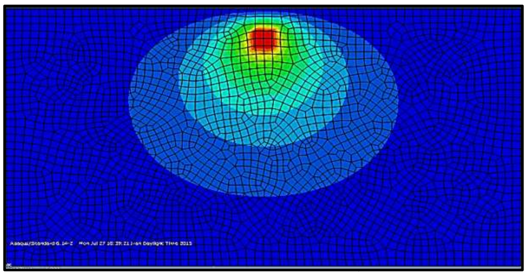

Fig. 8 Diffusion model conducted with ABAQUS for non-seismic mode, one layer profile and final

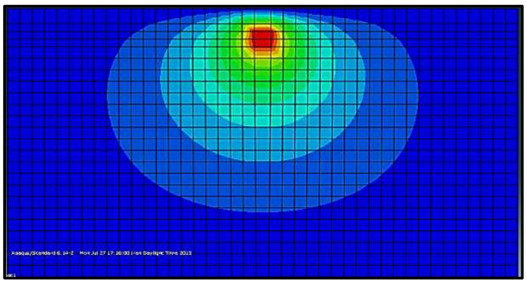

Fig. 9 Diffusion model conducted with ABAQUS for non-seismic mode, 3layer profile and final condition

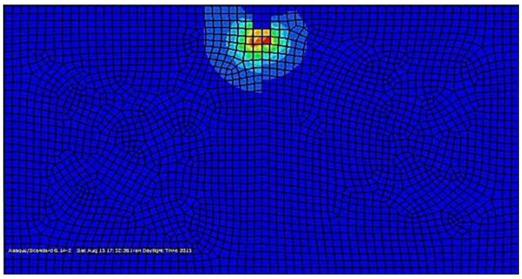

Fig. 10 Diffusion model conducted with ABAQUS for seismic mode, one layer profile and initial condition

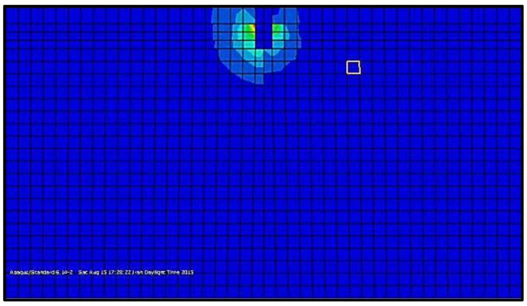

Fig. 11 Diffusion model conducted with ABAQUS for seismic mode, 3 layer profile and initial condition

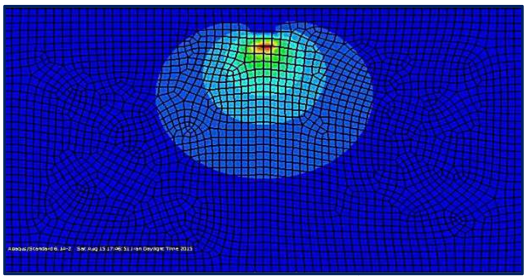

Fig. 12 Diffusion model conducted with ABAQUS for seismic mode, one layer profile and final condition

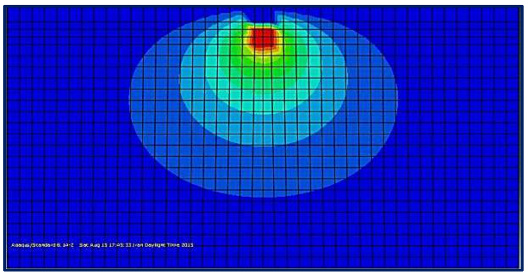

Fig. 13 Diffusion model conducted with ABAQUS for seismic mode, 3 layer profile and final condition

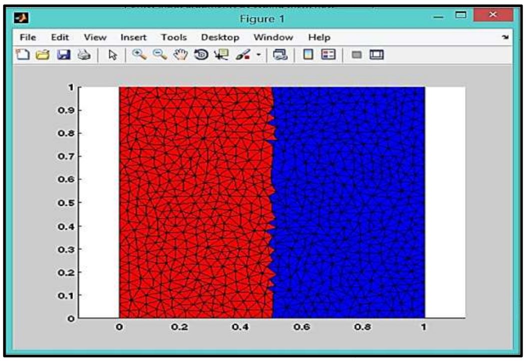

Fig. 14 Diffusion model conducted by MATLAB (before applying the Loma earthquake)

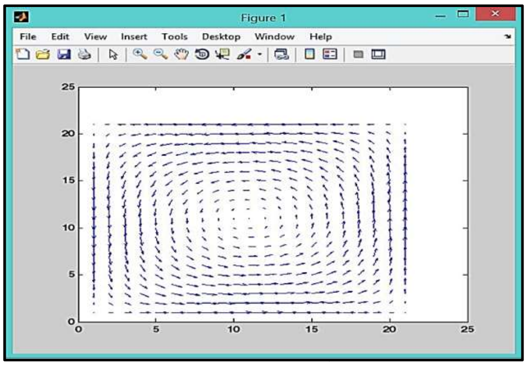

Fig. 15 Seismic velocity vectors produced by MATLAB for waste diffusion in seismic mode

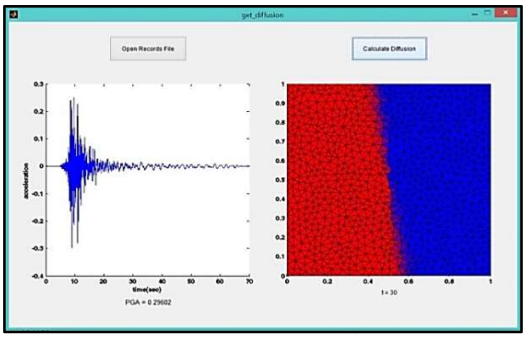

Fig. 16 Diffusion model conducted by MATLAB for

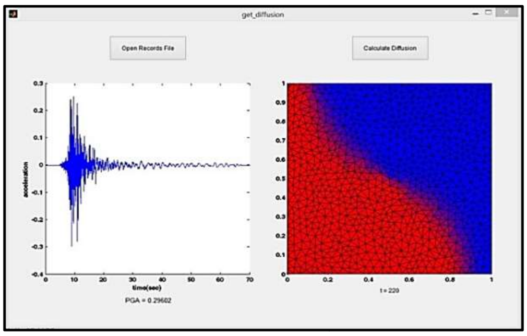

Fig. 17 Diffusion model conducted by MATLAB for

dynamic time of 30 seconds

dynamic time of 220 seconds

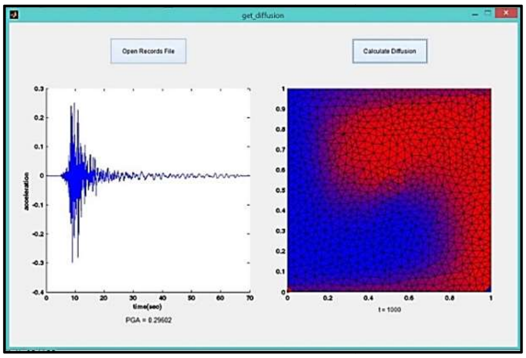

Fig. 18 Diffusion model conducted by MATLAB for dynamic time of 1000 seconds (final mode)

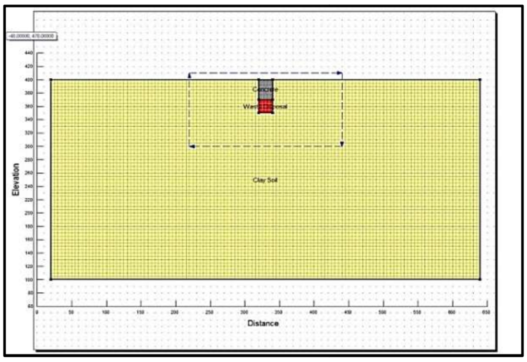

Fig. 19 Initial model of the soil and waste profile

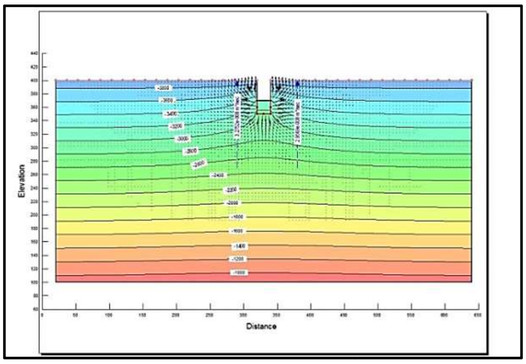

Fig. 20 Time counters of diffusion model conducted by seep/w and ctran/ w

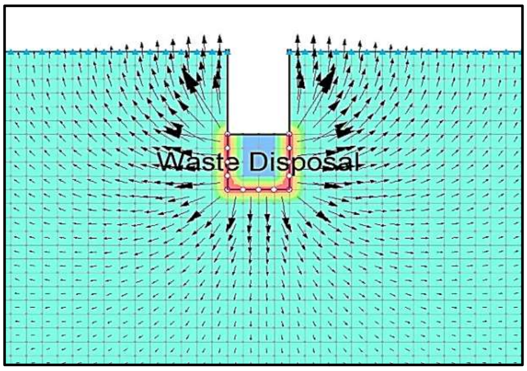

Fig. 21 final diffusion model of the soil profile conducted by seep/w and ctran/w

4. CONCLUSIONS

The soft wares which have been used in this study gave us verity of the results such as time counters of waste diffusion, the velocity of waste particles in diffusion model, and also the percentage of the hazardous waste during the time intervals. But qualitative comparison of these results shows that the modes of the diffusion given by different soft wares are similar to each other. For better evaluating, we analyze the problem from two aspects (seismic and non-seismic). The final result of this article can be this idea that to have better understand of waste diffusion in soil and rock media it is better to use set of the soft wares instead of one software and the comparing the results to gain a unit model can present the real condition. An important fact is that as we saw at pervious section, the normal PGA which is equal by 0.3(in this article) increased coefficient of diffusion up to 1.5 and we must consider this sudden increase as a caution when choosing the waste disposal place. As expected and also because of locating the waste disposal in uniform clay, the most percentage of diffusion model is extended in a close area(for this case,100 m) near the buried depth that make it easy to control the harmful effects at emergencies.by using suitable kind of clay which has lower factor of diffusion we can prevent arrival of radioactive waste to the surface before its half life time (i.e. the decay period of radioactive waste is less than the time which the waste needs to arrive the surface).As we saw in this article the concrete shield had a great effect in elongation of the distribution path so reinforcement concrete is recommended to be used as a shield even in seismic conditions.

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