Modeling Techniques for Geoenvironmental Engineering Problems

D. N. Singh[1] and B. Hanumantha Rao[2]

[1] Professor, Department of Civil Engineering, Indian Institute of Technology Bombay, Powai, Mumbai-400 076, dns@civil.iitb.ac.in
[2] Research scholar, Department of Civil Engineering, Indian Institute of Technology Bombay, Powai, Mumbai-400 076, hanuma_bendadi@iitb.ac.in

Abstract : Contamination of subsurface results in degradation of geomaterials (i.e., soils and rock mass), in the long run. This is mainly due to the presence of chemical and/or radiological materials in undesirable concentrations and at elevated temperatures. However, as contaminant-geomaterial interaction is an extremely slow and complex process, which primarily depends on their physical, chemical and mineralogical properties, it is quite difficult to study this interaction under laboratory or in situ conditions. In such a situation, accelerated physical modeling, using a geotechnical centrifuge, and finite element/difference based numerical modeling techniques are found to be quite useful.

This paper presents details of various modeling techniques developed by the researchers at the Indian Institute of Technology Bombay, Mumbai, India, for studying heat migration, flow and interaction (fate) of reactive and non-reactive contaminants in the geoenvironment, under saturated and unsaturated conditions. In addition, paper presents details of the technique that can be employed for determining susceptibility of a material to undergo physico-chemico-mineralogical alterations due to its interaction with contaminants.

Key words: Waste disposal, Contaminants, Geomaterials, Accelerated physical modeling, Numerical modeling

1. Introduction

Safe disposal of hazardous waste poses a big challenge to the planners and administrators, all over the world. The disposed off waste in the due course of time interacts with the rainwater or the fluctuating ground water table (Golubev and Garibyants, 1971; Chapman, 1987; IAEA, 1993) and gives rise to various complex geochemical processes and mechanisms that control its migration or transport in the soil-water or rock-water systems (Neretnieks et al., 1984; Lawrence, 1994; Byegard et al., 1998; Gurumoorthy and Singh, 2004). At the same time, high temperatures associated with these wastes tend to alter basic characteristics of the geomaterials (i.e., soils and rock mass), as well (Kolay and Singh, 2000; Krishnaiah et al., 2004). Hence, ascertaining the extent of changes undergone by these materials and how this interaction influences their over all engineering properties becomes essential.

The transport of contaminants is often predicted with the help of mathematical models (SKI, 1987), for which the input parameters have to be obtained by conducting either controlled field experiments or laboratory column tests (Naidu, 2006). Though, controlled field experiments are found to be more reliable, these tests are quite expensive, tedious and offer little control over the boundary conditions. On the other hand, laboratory column tests are cost effective and relatively easy to perform (Rajeev, 2002). However, both these methods

are not viable due to their limitations in modeling and simulating realistic prototype condition(s), since the time of interest may span decades of real time. To overcome these limitations, researchers (Schofield, 1980; Savvidou, 1988; Celorie et al., 1989; Hensley and Schofield, 1991; Mitchell, 1994; Zimmie et al., 1994; Hensley and Savvidou, 1995; Singh and Gupta, 2000; Manthena, 2001; Singh and Kuriyan, 2002; Rajeev, 2002; Gurumoorthy, 2002; Krishnaiah, 2003) have resorted to centrifuge modeling, which helps in simulating real life (prototype) conditions quite efficiently.

With this in view, utility of a geotechnical centrifuge to model contaminant transport in soils (Rajeev, 2002; Sreedeep et al., 2003) and the intact and fractured rock mass (Villar and Merrifield, 1992; Gurumoorthy and Singh, 2004) has been demonstrated, in the present study. In addition, studies were conducted to model migration of heat in soils (Manthena and Singh, 2001; Krishnaiah and Singh, 2004a,b). Based on the centrifuge results, validity of 'modeling of models' has been shown and potential of a small geotechnical centrifuge, as a research tool has been established. The results were compared with those obtained from the finite element based models (viz., SEEP/W and CTRAN/W) for contaminant transport (Sreedeep et al., 2003) and ANSYS 6.0 for heat migration (Krishnaiah, 2003) in soils and an excellent matching between the results has been noted. However, to model contaminant and heat migration in rocks, the closed-form solutions were developed and their validity has been checked.

In addition, paper presents details of the technique that can be utilized for determining susceptibility of a material (in the present study fly ash has been considered) to undergo physico-chemico-mineralogical alterations due to its interaction with contaminants.

It has been demonstrated that such modeling exercises would be of great help in understanding and simulating response of the geomaterials in real life and hence in designing efficient barrier/containment and backfill systems.

2. Experimental Investigations

2.1 Accelerated Physico-chemico-mineralogical Modeling

During interaction of the waste (and geomaterials) with water, under elevated temperatures, the hydroxides leach out of the matrix and their prolonged interaction alters the physical, chemical and mineralogical characteristics of these materials. A good example of this type of interaction is ash-water interaction, as elaborated in the following.

A common method of disposing ash is its wet disposal, where the ash is mixed with water to make slurry and is disposed off in the ash ponds or lagoons (Theis and Gardner, 1990; Lister and Peterson, 1996; Sharma, 1996). Such a disposal system causes ash, and the alkalis present in it, to interact with water over a period of time and may lead to the formation of ash zeolites (Singh and Kolay, 2002; Kolay et al., 2001; Kolay and Singh, 2001a, b). As such, it would be interesting to study the effect of this interaction (i.e., formation of zeolites, which is also termed as zeolitization of the ash) on physical, chemical and mineralogical characteristics of the ash (Kolay and Singh, 2001b). As geotechnical properties of a material depend on these characteristics, the influence of zeolitization on these properties of the ash must also be investigated (Grutzeck and Siemer, 1997; Steenbruggen and Hollman, 1998). Such investigations are also essential for the bulk utilization of the lagoon ash, in particular as a fill material, where properties like compaction, consolidation, hydraulic conductivity and its shear strength are very important (Kolay and Singh, 2001a, b).

Lagoon ash sample from the ash disposal pond of Koradi Thermal Power Plant (KTPP), Nagpur, Maharashtra, India, was collected for the present study. Ash sampling was done randomly, in four batches during a span of seven days, so as to minimize the effect of heterogeneity. Later these batches were mixed together to prepare a representative sample of the ash. This sample, denoted as the original lagoon ash, OLA, was subjected to a series of

tests for determining morphological characteristics (by employing a scanning electron microscope, SEM), chemical characteristics (by conducting X-Ray Fluorescence studies) and mineralogical characteristics (by conducting X-Ray Diffraction studies).

The OLA was activated by alkali treatment, so as to simulate its interaction with water and the changes it undergoes in the process of slurry disposal. 160 ml alkali solution (NaOH and KOH) of 0.5, 1.0, 2.0 and 3.5 M was used for activating the ash sample, in an open system, maintaining solid liquid ratio equal to 0.125 g/l. The activation temperature of approximately 100°C was maintained by using a water-bath and a reflux system. The process time varied from 12, 24, 36 and 48 h, respectively. At the end of these activation periods, the ash sample was filtered and repeatedly washed with distilled water. It has been observed that KOH activation does not result in the formation of zeolites and the ash sample treated with 1 M NaOH for 24 hours results in the formation of NaP1 and Hydroxy-sodalite zeolites (Henmi, 1987; Kolay et al., 2001). This activated ash sample has been designated as ALA.

Fig. 1 depicts SEM micrographs of OLA and ALA samples. These micrographs indicate the presence of particles with different shapes viz. spherical, hollow (cenosphere), broken, plerosphere (i.e. a sphere within another sphere), tubular and some other irregular shaped particles in the OLA sample. However, it can be noticed from SEM micrographs of ALA sample that due to the alkali activation some overgrowth on the surface of the ash particles takes place. It has been noticed that the alkali activation is responsible for etching (and hence dissolution) of the silica present in the ash. The alkali activation of the OLA results in an increase in its specific gravity by 12 to 25% with different strength of NaOH and time periods. The specific surface area of the OLA sample is noticed to increase by 0.7 to 143% with different strength of NaOH and activation time periods. The void ratio and porosity of the ALA sample is noticed to increase by about 23 to 48% and 8 to 23%, respectively, as compared to the OLA sample (Singh and Kolay, 2002a).
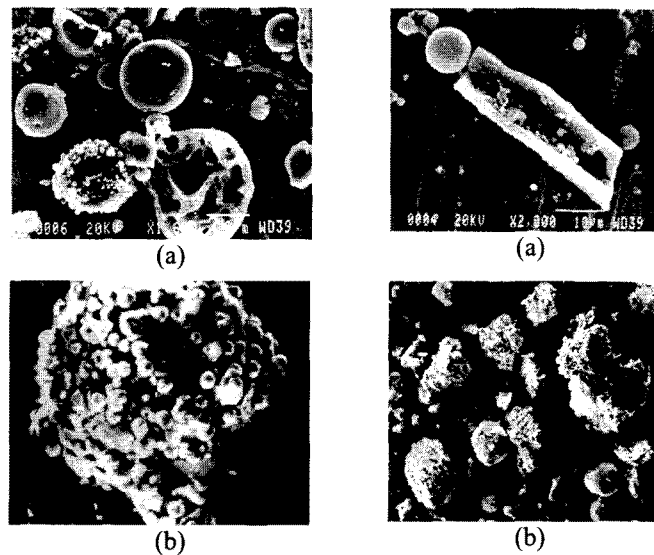

(a)   (a)

(b)   (b)

Fig. 1. SEM micrographs of (a) OLA and (b) ALA samples

The alkali activation results in a decrease in maximum dry density by 8.5%, as depicted in Fig. 2. However, the water absorption capacity of the ash is noticed to increase by almost 33%. This results in an increase of the hydraulic conductivity of the ash by approximately 35%, at the optimum moisture content, as depicted in Fig. 3. Alkali activation also leads to an increase in the shear strength of the ash, as depicted in Fig. 4 (Singh and Kolay, 2002b).
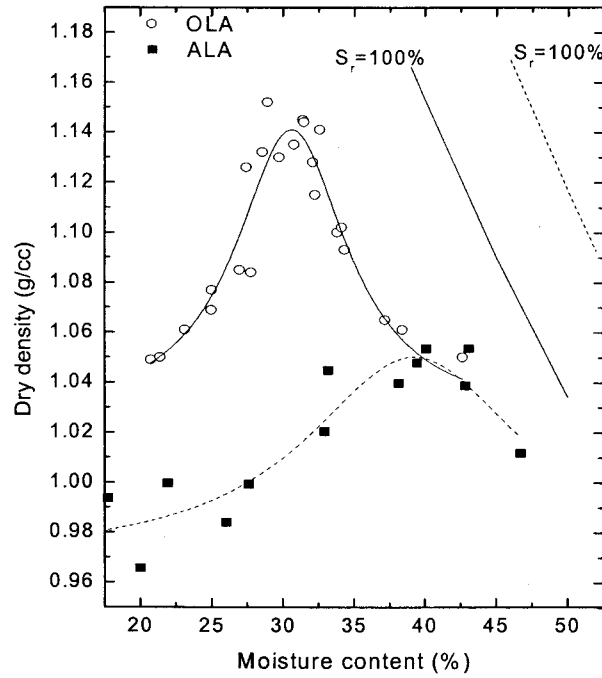
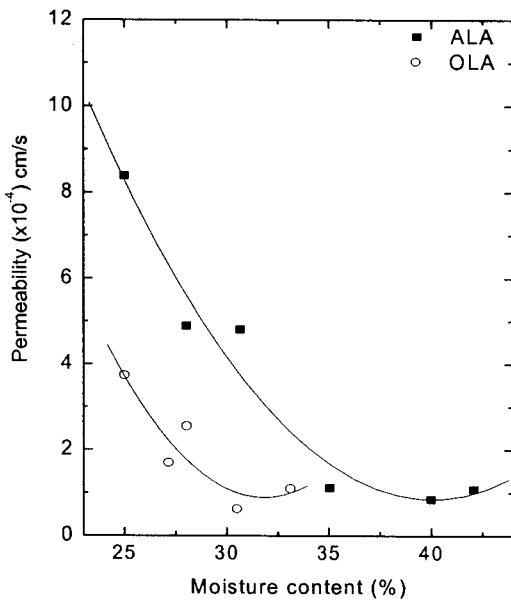Fig. 2. Compaction characteristics for OLA and ALA samples

Fig. 3. Variation of permeability with moisture content for the OLA and ALA samples
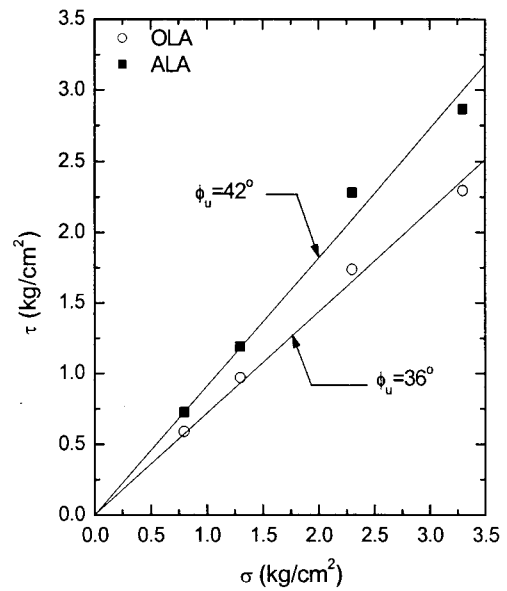
Fig. 4. Shear strength envelopes for OLA and ALA samples

2.2 Accelerated Physical (Centrifuge) Modeling

Details of the geotechnical centrifuge employed for these studies are listed in Table 1. The silty soil used in the study belongs to SM classification (Krishnaiah, 2003) while the rock mass used in the study is a Charnockite type (AMD, 1995). The rock mass exhibits porosity of 0.32% and density of 2.58 g/cc (Gurumoorthy, 2002).

Table 1. Details of the geotechnical centrifuge used in the study

Parameter	Value
Type	Swinging buckets on both sides of the arm
Arm radius (mm)	200
Max. outer radius (mm)	315
Centrifuge range (rpm)	250-1000
Max. acceleration (g)	300
Spin-up time (s)	20

2.2.1 Contaminant Migration in Soil

As depicted in Fig. 5, the centrifuge test setup consists of 2 detachable concentric Perspex cylinders that are mounted on a Perspex base plate. The graduated inner cylinder is 60 mm inner diameter and 150 mm in length, provided with 5 sets of brass electrodes, (15 mm c/c spacing), for monitoring contaminant migration in the soil. The outer cylinder is 112 mm inner diameter and 50 mm long. A thin perforated Perspex plate is kept at the bottom of the sample to enable outflow of water or the contaminant percolating through the soil sample. An adequate amount of the air-dried soil was mixed with varying moisture content, and stored for 24 h in airtight bags, for its preconditioning and maturing. The matured soil was compacted in three layers in the Perspex cylinder using a flat bottom hand rammer to achieve 70 mm long sample of the required compaction density, γ_d, and the water content, w, as listed in Table 2.

Table 2. Details of the samples used in the study

Sample	γ_d (g/cc)	w (%)
A	1.77	9.67
B	1.83	12.23

Migration of contaminant in these samples, during centrifugation, was monitored with the help of a contaminant detector and a datalogger (Rajeev, 2002; Rajeev and Singh, 2004). Prior to the start of the experiment, the background Cl⁻ concentration of the sample was measured. 35 mm high column of 1 M NaCl solution, which acts as a model contaminant, was poured on the top of the soil sample, as depicted in Fig. 5.
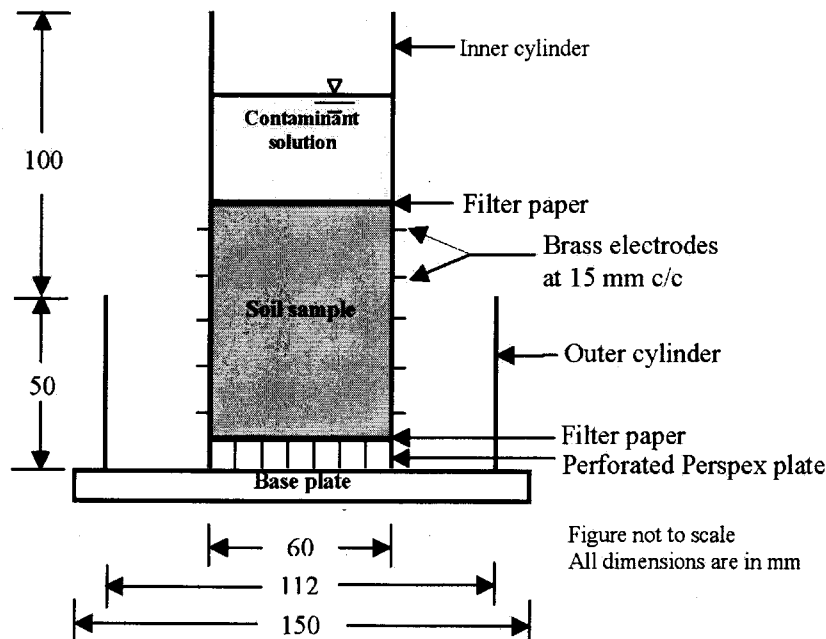

Fig. 5. The centrifuge test setup

The space between the soil sample and the Perspex cylinder was sealed with an epoxy to avoid any preferential flow of the NaCl solution. This setup was placed in the centrifuge and connected to the contaminant detector (Rajeev and Singh, 2004) and a datalogger. Tests were conducted at an acceleration level of 100-g, which would yield prototype times of 90 and 153 days and the results are depicted in Fig. 6.
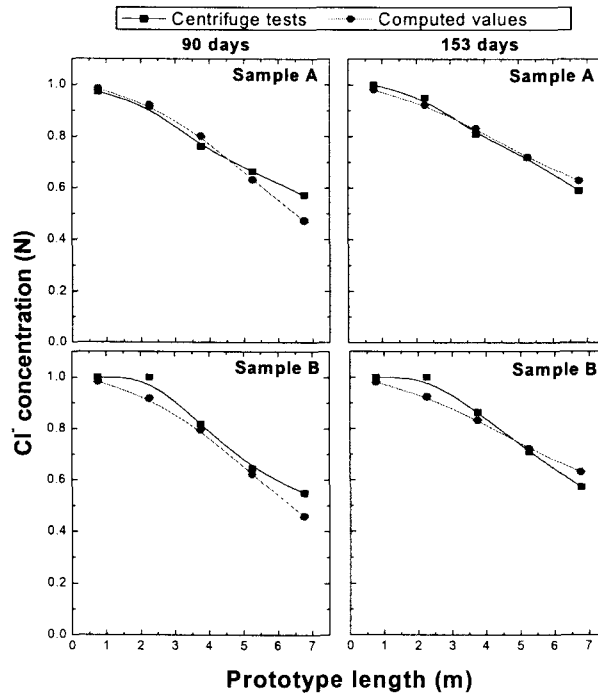

Fig. 6. Variation of the Cl⁻ concentration along the length of soil samples (at N=100)

Fig. 6 also presents results obtained from the SEEP/W and CTRAN/W, finite element (FEM) based computer codes. The data presented in Table 3 was employed for this analysis. It can be noted from Fig. 6 that the centrifuge results match very well with the computed results. However, a small discrepancy in the results can be attributed to non-uniform compaction of the soil sample along its length.

Table 3. Data used for the FEM analysis

Parameter		Value
Number of elements		241
Diffusion coefficient (m^2/s)		2.0E-09
Boundary conditions:		
Pressure head (m)	@ top of the sample	3.5
	@ bottom of the sample	0.0
Mass flux, Q_d, (kg/s)		>0

2.2.2 Heat Migration in Soils

The thermal resistivity of silty soil can be measured with the help of a laboratory thermal probe, which works on the principle of "transient heat method" (Hooper and Lepper, 1950). The thermal probe approximates a line heat source of input Q per unit length, of constant strength, in an infinite homogeneous medium, initially at uniform temperature. The probe consists of a nichrome heater wire (0.042 Ω/cm resistance) inserted in a 95 mm long copper

tube and of 6 mm external diameter. When a constant current is passed through the heater wire, the rate of heat transfer from the probe in the medium in which it is inserted, can be determined with the help of a thermocouple (Type-T, copper constantan) attached to the inner surface of the probe. The change in temperature of the probe depends on thermal conductivity of the medium and the following equation can be used to describe the heat migration mechanism:

$$\frac{\partial \theta}{\partial t} = \kappa \left[\frac{\partial^2 \theta}{\partial x^2} + \frac{1}{x} \frac{\partial \theta}{\partial x} \right] \tag{1}$$

where θ is the temperature of the medium, t is the time of heating, κ is the thermal diffusivity ($=k/\gamma C_p$), k is the thermal conductivity of the soil, C_p is the specific heat of the soil, γ is the unit weight of the soil and x is the radial distance from the heat source.

Eq. 1 can be solved for a particular case of temperature difference due to the heat input of Q ($=i^2.\xi$) where ξ is the resistance per unit length of the probe and i is the strength of the current in Amp. Thus the temperature rise between the time interval t_1 and t_2 is given by:

$$\Delta \theta = \left[\frac{Q}{4\pi} \right] . \frac{1}{k} \log_e \left[\frac{t_1}{t_2} \right] \tag{2}$$

To obtain the thermal resistivity, R_T ($=1/k$) of the material, Eq. 2 can be rewritten as:

$$R_T = \frac{4\pi}{2.303Q} . \frac{\Delta \theta}{\Delta \log_e t} \tag{3}$$

The probe was calibrated by using standard liquid glycerol for which the thermal resistivity value is 349 °C-cm/W (Singh et al., 2003; Krishnaiah and Singh, 2004; Krishnaiah et al., 2004).

Special instrumentation was developed for modeling heat migration in soils, in a centrifuge as depicted in Fig. 7 (Manthena and Singh, 2001; Krishnaiah, 2003).
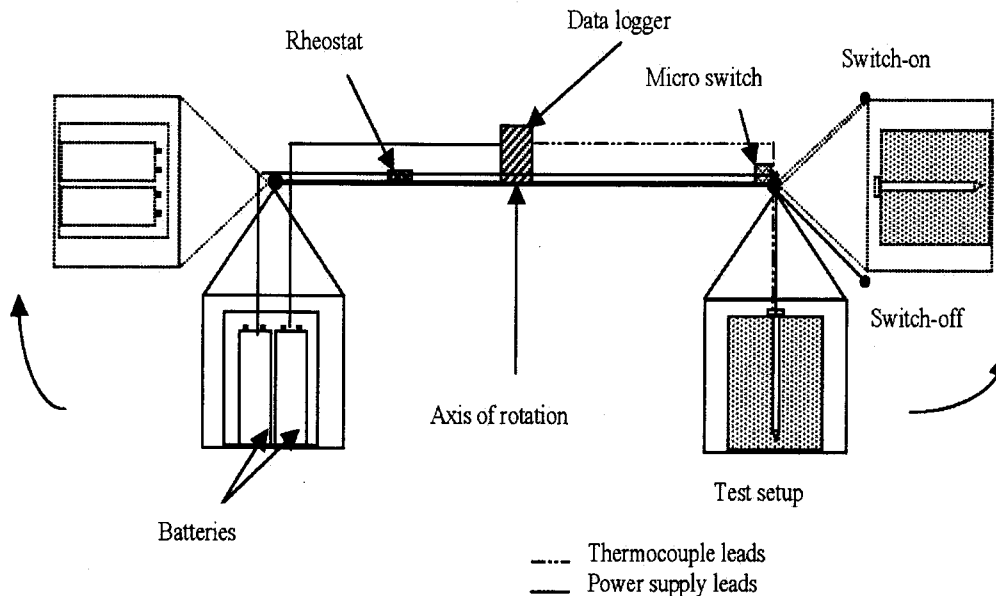

Fig. 7. Centrifuge setup for modeling heat migration in soils

Such a setup facilitates measurement of the probe temperature, and the input voltage, during centrifugation of the sample. Two rechargeable 6 V lead-acid batteries, which also act as counter weights to the soil sample, were used as the power source for heating the probe and for the datalogger. A rheostat was used to regulate the input power supply to the probe. The air-dried soil was compacted to different dry densities, γ_d (=1.2, 1.3, 1.4 and 1.5 g/cc) in a Perspex cylinder, imparting 20 blows to each soil layer using a flat bottom hand rammer, to achieve 11 cm long soil sample. Thermal resistivity tests were conducted and variation of temperature with time was recorded for each sample. Typical results for the soil samples compacted at γ_d=1.2 g/cc are depicted in Fig. 8, corresponding to 1-g and N-g tests (N=50, 100, 125 and 150). Using Eq. 3 and the discussion presented above, R_T, values for the soil were obtained and are plotted as depicted in Fig. 9.
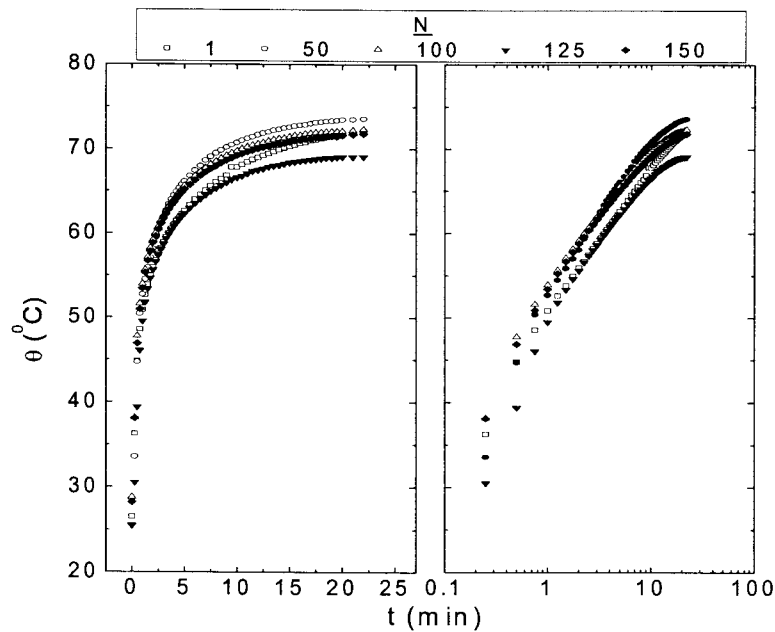

Fig. 8. Typical response of the thermal probe (for soil sample with γ_d=1.2 g/cc)
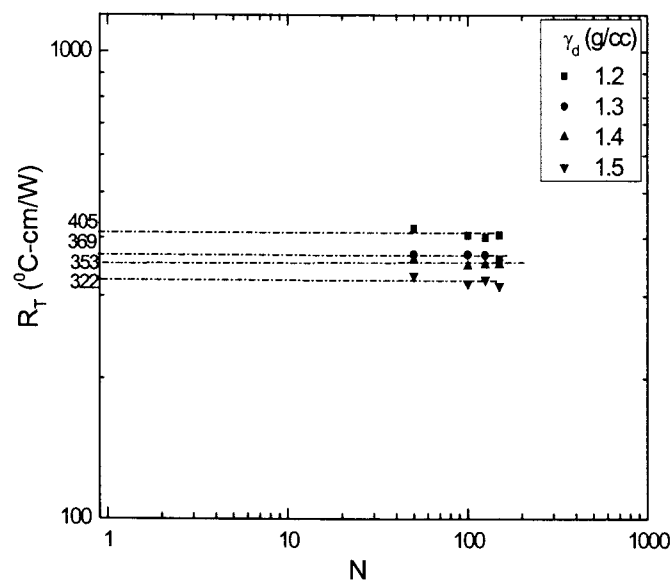

Fig. 9. Modeling of models for thermal resistivity

As depicted in Fig. 9, R_T values have been obtained corresponding to 1-g by extrapolation of the centrifuge results. The R_T values corresponding to γ_d=1.2, 1.3, 1.4 and 1.5 g/cc are noted to be equal to 405, 369, 353 and 322 ^{0}C-cm/W, respectively. These values when compared with the measured R_T values at 1-g (425 ^{0}C-cm/W) exhibit a maximum error of 6%. This demonstrates that the modeling of models is valid. In other words, the study reveals that the thermal resistivity being a material property remains unaltered in an accelerated environment, as reported in the literature (Manthena, 2001; Manthena and Singh, 2001).

From Fig. 10, it can be observed that in general as γ_d increases, R_T decreases for all N values, and beyond γ_d=1.6 g/cc there is no influence of N on the R_T value (which is equal to 315 ^{0}C-cm/W). These trends are consistent with the results reported in the literature (Rao and Singh, 1999).
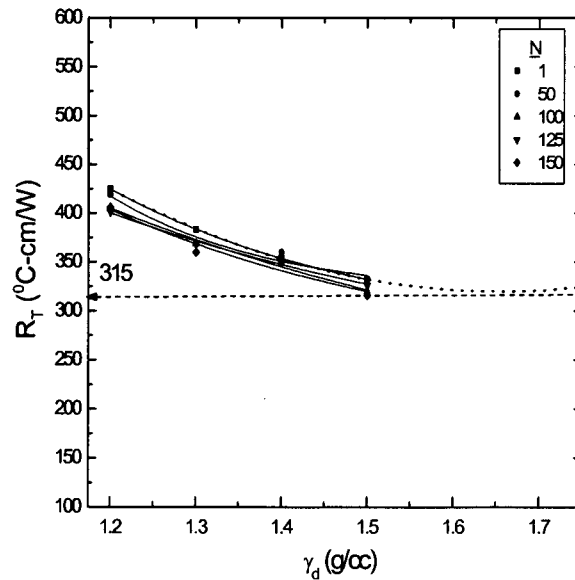

Fig. 10. Variation of R_T with γ_d for the silty soil

Results from ANSYS 6.0 are compared with those obtained from the laboratory (1-g) experiments, as depicted in Fig. 11, for the dry soil sample (γ_d=1.2 g/cc). In the figure, r depicts the radial distance of the thermocouple from the centre of the probe.
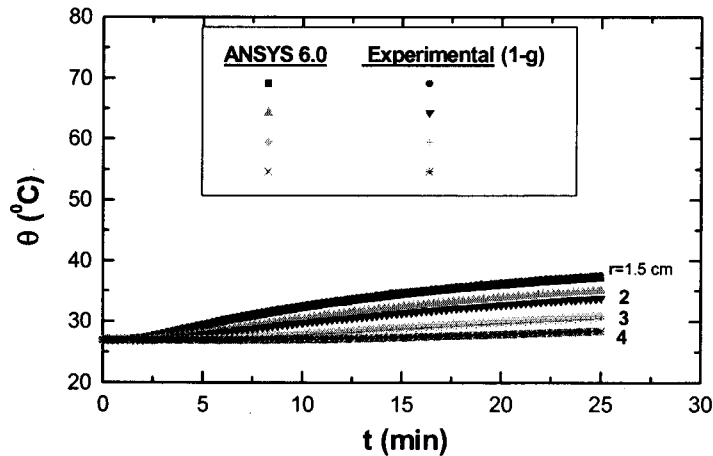

Fig. 11. Results for heat migration in the soil sample

Fig. 11 also indicates that the finite element model developed by the authors is a generalized model and hence it can be used to study heat migration in geomaterials, quite well. Attempts were also made to use the results obtained from this model to verify validity of scale factor for time, by using the following relationship:

$$\Lambda = \frac{\log_{10}\left(\dfrac{t_p}{t_m}\right)}{\log_{10}(N)} \tag{4}$$

Using Eq. 4, values of Λ were computed for N=50, t_m=10 min and different values of r, as depicted in Table 4. It can be noted that the value of Λ is very close to 2, which indicates that the migration of heat occurs N^2 times faster in a model as compared to its prototype (Arulanandan et al, 1988; Krishnaiah and Singh, 2004).

Table 4. Values of the time scale factor for centrifuge tests at N=50

θ (°C)	Finite Element Model		Centrifuge tests		Λ
	r_p (cm)	t_p (min)	r_m (cm)	t_m (min)	
32.0	75	12905	1.5	10	1.83
28.8	100	15485	2.0	10	1.88
26.8	150	17105	3.0	10	1.90

2.2.3 Contaminant Migration in Rock Mass

Centrifuge tests were conducted on 3 mm intact and 60 mm fractured rock mass using the diffusion cells depicted in Figs. 12 and 13, respectively (Gurumoorthy and Singh, 2004).

0.1 M NaCl solution was used as the model contaminant (the source solution concentration C_0, was found to be 3546 ppm with respect to the Cl⁻) to study the diffusion of contaminants in the intact and fractured rock mass. The concentration of Cl⁻ (C_t) diffusing in the rock mass was determined by the Ion Chromatography (IC) technique and is expressed as milligrams/litre (mg/l). The obtained C_t values when normalized with C_0 and plotted as C_t/C_0 versus t yield the diffusion characteristics of the Cl⁻, as depicted in Fig. 14. It can be noted from the figure that these characteristics are linear. For obtaining D_i the methodology discussed in the following was adopted:

$$D_i \frac{\partial^2 C(x,t)}{\partial x^2} = \alpha \frac{\partial C(x,t)}{\partial t} \tag{5}$$

where D_i is the diffusion coefficient of the ion, x is the distance and α is the rock capacity factor (or volume factor). Eq. 5 can be solved analytically with the help of following initial and boundary conditions (Wen et al., 1997):
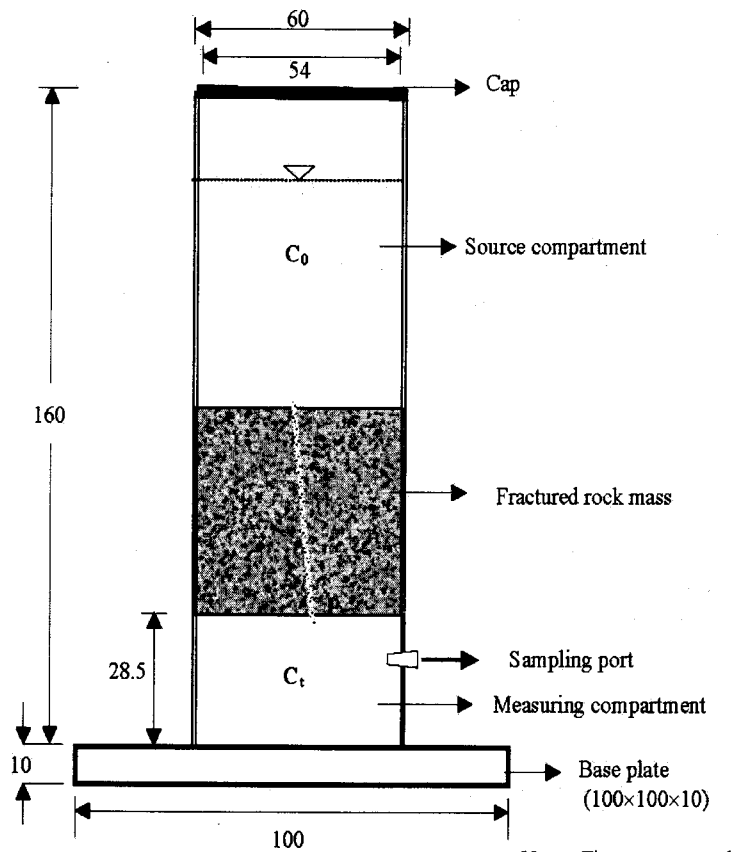
$$C(x,t)|_{t=0} = 0 \quad \text{for } x > 0 \quad \dots\dots\dots(a)$$

$$C(x,t)|_{x=0} = C_0 \quad \text{for } t \geq 0 \quad \dots\dots\dots(b) \tag{6}$$

$$\frac{\partial C(x,t)}{\partial t}\bigg|_{x=L} = 0 \quad \text{for } t > 0 \quad \dots\dots\dots(c)$$

if the concentration of a contaminant at x=L is such that; C(L, t)<<C_0, and t is large enough, then the solution of the Eq. 4 can be represented as:
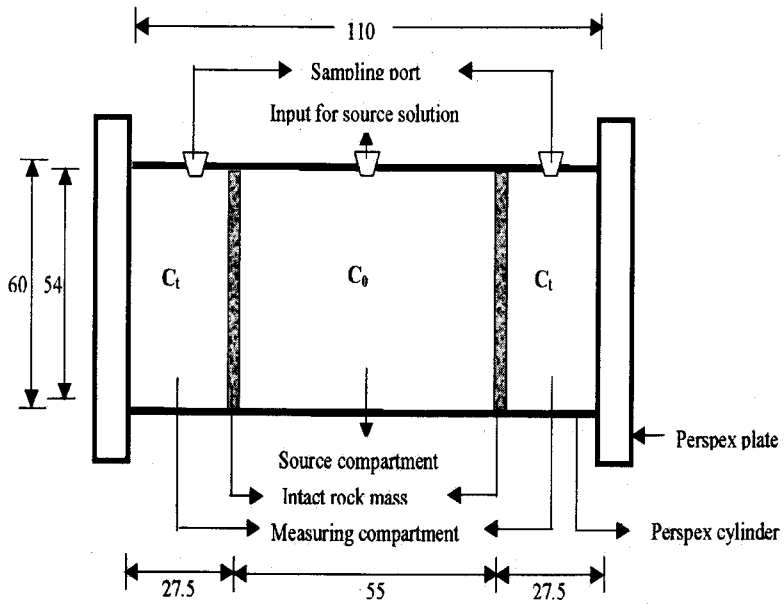
Fig. 12. Diffusion cell used for the intact rock sample
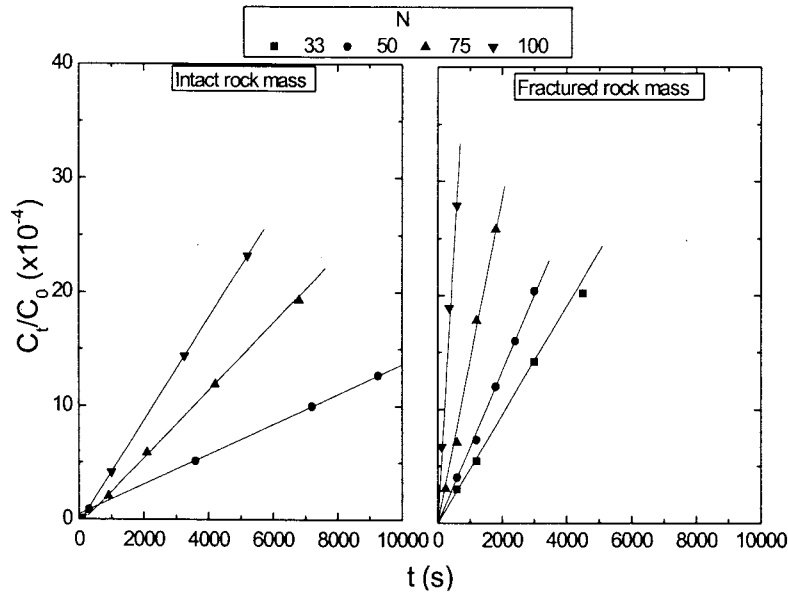

Fig. 13. Diffusion cell used for the fractured rock sample

Fig. 14. Diffusion characteristics of the Cl⁻ for the intact and fractured rock samples

$$\frac{C_t}{C_0} = \left(\frac{D_i.A}{L.V} t - \frac{\alpha.A.L}{6V} \right) \tag{7}$$

where A and L are the area and thickness of the rock mass, respectively. For the fractured rock mass, A (=aperture in μm $\times$ 0.0545 m) is the area of the fracture and L (= 0.06 m) is the length of the fracture. V is the volume of the solution in the measuring compartment.

Eq. 7 represents a straight line with slope, s:

$$s = \left(\frac{D_i.A}{L.V} \right) \tag{8}$$

$$\text{or,} \qquad D_i = \left(\frac{s.L.V}{A} \right) \tag{9}$$

Scaling of diffusion number π_4, as defined by Arulanandan et al. (1988) leads to similarity of diffusion processes in the model and its prototype. π_4, can be expressed as:

$$\pi_4 = (D_i.t/L^2) \tag{10}$$

Eq. 10 indicates that for an identical contaminant and for an identical rock mass, the following condition must be satisfied:

$$D_{i(m)} = D_{i(p)} \tag{11}$$

where m and p represents model and the prototype, respectively.

As such, to maintain similarity of π_4, the following condition must be valid:

$$t_m = N^{-y} t_p \tag{12}$$

where t_p and t_m correspond to the diffusion time for the prototype and its model, respectively, and y is the time factor.

Following this methodology, D_i values for the Cl⁻ for the intact and fractured rock mass were computed and are listed in Table 5.

Table 5. Experimental values of the diffusion coefficient $(\times 10^{-12} \, m^2/s)$

Rock mass	N= 1	33	50	75	100
I	0.12	-	8.64	7.59	11.61
F	350	44370	42650	47390	50960

- not available; I: Intact; F: Fractured

It can be observed from Table 5 that the order of magnitude of D_i for intact and fractured rock mass, corresponding to the conventional tests and various acceleration levels, N, is almost same. A small variation in the absolute value of D_i can be ignored and may be attributed, mainly, to non-identical porosity of the rock samples, which were used in the study. This demonstrates validity of Eq. 10 for the intact and fractured rock mass. D_i values for the intact rock mass are also found to be matching very well with the results reported in the literature $(0.2\text{-}2\times10^{-12} \, m^2/s)$ by Vesa et al. (1997). Unfortunately, similar comparison for the fractured rock mass could not be done due to the lack of results reported in the literature. However, these values are noted to be higher than the free diffusion coefficient of Cl⁻ $(=5\times10^{-9} \, m^2/s)$ in the aqueous media (SKI, 1987). To demonstrate the utility of the centrifuge for modeling the diffusion time of Cl, in the intact as well as the fractured rock mass, the time required for $C_t/C_0=20\times10^{-4}$ was obtained from Fig. 13 and was plotted as depicted in Fig. 15.
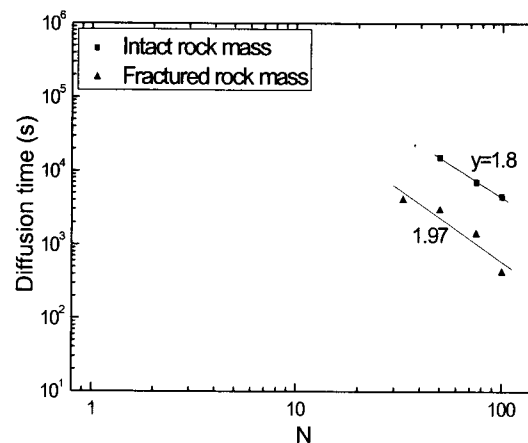

Fig. 15. Modeling of models for the diffusion time for the Cl⁻

The slope of the relationship (the absolute value of 'y', as depicted by Eq. 12) is found to be equal to 1.8 and 1.97 for the intact and fractured rock samples, respectively. This indicates that scaling factor for the diffusion of Cl⁻ in the rock mass can be assumed to be 2. This is consistent with the diffusion time scale factor reported in the literature (Arulanandan et al., 1988). This demonstrates the usefulness of a geotechnical centrifuge for modeling contaminant diffusion in the rock mass.

3. Concluding Remarks

The usefulness of modeling in studying and simulating various geoenvironmental problems has been demonstrated in this paper. The potential of accelerated physical modeling and numerical modeling techniques for contaminant and heat migration in geomaterials, in extremely short duration, has been brought out very clearly. In addition, the potential of the

technique that can be employed for determining susceptibility of a material to undergo physico-chemico-mineralogical alterations due to its interaction with contaminants has also been demonstrated.

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