International Journal of Engineering and Advanced Technology (IJEAT)
ISSN: 2249-8958 (Online), Volume-8 Issue-4, April 2019

Using Numerical Model to Evaluate Pozzolanic Activity of Natural Pozzolan in The Soil Stabilization Process

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Abstract*: *Natural pozzolan is one of raw materials that is regularly used in the soil stabilization process. The paper uses thermodynamic model to evaluate pozzolanic activity of natural pozzolan. Based on mineralogical composition of two types natural pozzolan: one of Daknong-Vietnam and another one of Bigadiç-Turkey, the thermodynamic model can simulate chemical composition of pore solution, mineral precipitation quantity. From this simulation, numerical quantity calcium silicate hydrated C-S-H and calcium aluminate silicate hydrated C-A-S-H can be calculated. Different cases of mix design: soil/pozzolan/lime are set up. In all of the cases, a comparison of quantity C-S-H and C-A-S-H between of two natural pozzolan is carried out to evaluate the pozzolanic activity of the each natural pozzolan. Thermodynamic model seems to be considered as a tool to evaluate pozzolanic activity of natural pozzolan.

Index Terms*: *Numerical model, Activity of natural pozzolan, Soil stabilization process, Daknong Vietnam.

I. INTRODUCTION

Economic development demands necessary new infrastructure construction. That leads to increase use materials construction. However, purpose to reducing impact of the greenhouse CO2 gas effect from construction materials production process, therefore, using of raw materials to replace industrial materials is necessary to protect the environment. Natural pozzolan is one of the most used raw materials as a binder in the soil stabilization process in construction. In fact, there exist many types of natural pozzolan with different activity levels. Each type of pozzolan used leads to different properties of the stabilized soil, affecting the quality of the construction. Therefore, the choice of pozzolan is very important. The geochemical model was proposed [1] and validated to find mix design of stabilized soil using natural pozzolan. Therefore, the geochemical model is recommended for pozzolanic activity evaluation of natural pozzolan. Based on the evaluation, appropriate selection pozzolan is feasible. In first part, several main equations of geochemical model are presented. In next section, equations of chemical reaction system of stabilized soil using pozzolan, cement and lime are introduced as well as the input parameters of geochemical model such as mineral composition of natural soil, mineral composition of natural pozzolan Daknong [1] and Bigadiç [2], as well as mix-designs. Comparing results of the two types of pozzolan are performed in next section. Conclusions and perspectives are also given in the last part of the article

II. MODELLING APROACH

A. Thermodynamic equilibrium

The interaction between the ionic species and the mineral species leads to precipitation/dissolution of minerals. The mineral saturation ratio Ω_m can be expressed as:

$$\Omega_m = K_{s,m}^{-1}\prod_{j=1}^{N_c}(\gamma_j C_j)^{\nu_{mj}} \qquad m = 1, \ldots, N_p \tag{1}$$

Where m is the indice of the mineral species, $K_{s,m}$ is the equilibrium constant.C_j is the molar concentration of primary species in the solution (mol.kg-1) i.e. the species that are supposed to move in the solution/ Other ions (often more complex) are taken into account when ionic complexations are calculated (see equation 3). ν_{mj} is the stoichiometric coefficient of the primary species, γ_j is the activity coefficient of the ion j , N_c , N_p are the number of corresponding primary species and mineral species. The state of equilibrium (or disequilibrium) of mineral species in the solution is controlled by the mineral saturation index IS_m, as follows:

$$IS_m = \log \Omega_m \tag{2}$$

For a given mineral species, the solution is in equilibrium with the mineral species if $IS_m = 0$. The solution is under-saturated and the mineral species can still dissolve if $IS_m < 0$. Finally, the solution is super-saturated and the mineral species may be precipitated if $IS_m > 0$. Aqueous complexes are formed by interactions between primary species in the solution. These reactions are assumed to be at local equilibrium. By using the mass action law, the concentration of aqueous complexes can be expressed as a function of the concentration of primary species, as follows:

$$C_i = K_{c,i}^{-1}\gamma_i^{-1}\prod_{j=1}^{N_c}(\gamma_j C_j)^{\nu_{ij}} \qquad i = 1, \ldots, N_x \tag{3}$$

Manuscript published on 30 April 2019.
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where C_i is the molal concentration of the aqueous complexes i ($mol.kg^{-1}$). γ_i, γ_j are the activity coefficients. $K_{c,i}$ is the equilibrium constant of aqueous complexation. N_x is the number of aqueous complexes considered in the solution. Thermodynamic database includes these parameters, the thermodynamic database THERMODDEM of Blanc et al [3] is applied in this paper.

B. Chemical reaction and required input data

Mineralogical composition of the initial materials: Soil, lime, volcanic ash was identified by powder X-ray diffraction (XRD). The Bogue calculation to determine the unhydrated clinker phases in the ordinary Portland cement (OPC) is more detailed in the Tran's work [4]. The initial mineralogical composition of the mixture is given in **Error! Reference source not found.**

Table 1. Mineralogical composition of the initial materials

Material	Phase	Formula	Composition (g/100g)
Soil	Quartz	SiO_2	4
	Kaolinite	$Al_2Si_2O_5(OH)_4$	23
	Gibbsite	$Al(OH)_3$	61
Lime	Lime	CaO	66
	Portlandite	$Ca(OH)_2$	16
	Calcite	$CaCO_3$	9
	Periclas	MgO	3
	Quartz	SiO_2	1
Natural pozzolan Daknong	Diopside	$CaMg(SiO_3)_2$	29
	Forsterite	Mg_2SiO_4	23
	Cristobalite	SiO_2	1
	Albite	$NaAlSi_3O_8$	27
	Quartz	SiO_2	4
Natural pozzolan Bigadiç	Quartz	SiO_2	0.5
	Clinoptilolite	$Ca_{0.55}(Si_{4.9}Al_{1.1})O_{12}.3.9H_2O$	82.9
	Opal	$SiO_2.nH_2O$	6.1
	Biotite	$Fe_3(OH)_2(Si_3AlO_{10})$	2.1
	Albite	Ca_3SiO_5	6.5
Unhydrated Portland cement	Alite (C3S)	Ca_3SiO_5 or ($3CaO.SiO_2$)	16.75
	Belite (C2S)	Ca_2SiO_4 or ($2CaO.SiO_2$)	54.45
	Aluminate (C3A)	$Ca_3Al_2O_6$ or ($3CaO.Al_2O_3$)	14.08
	Ferrites (C4AF)	$Ca_4Al_2Fe_2O_{10}$ or ($4CaO.Al_2O_3.Fe_2O_3$)	8.52
	Gypsum	$CaSO_4.2H_2O$	1.40

The chemical reaction system of soil stabilization process is presented in the table 2, as well as the equilibrium constant at ambient environment 25°C, 1 atm

Table 2. Chemical reaction and equilibrium constant at 25°C, 1 atm.

Chemical reaction	log K
$Quartz + 2H_2O = H_4SiO_4$	-3.74
$Kaolinite + 6H^+ = 2Al^{3+} + 2H_4SiO_4 + H_2O$	6.47
$Gibbsite + 3H^+ = Al^{3+} + 3H_2O$	7.74
$Hematite + 6H^+ = 2Fe^{3+} + 3H_2O$	-0.04
$Goethite + 3H^+ = Fe^{3+} + 2H_2O$	0.36
$Lime + 2H^+ = Ca^{2+} + H_2O$	32.70
$Portlandite + 2H^+ = Ca^{2+} + 2H_2O$	22.81
$Calcite + H^+ = Ca^{2+} + HCO_3^-$	1.85
$Periclas + 2H^+ = Mg^{2+} + H_2O$	21.59
$Diopside + 4H^+ + 2H_2O = Ca^{2+} + Mg^{2+} + 2H_4SiO_4$	21.73
$Forsterite + 4H^+ = 2Mg^{2+} + H_4SiO_4$	28.60
$Cristobalite + 2H_2O = H_4SiO_4$	-3.16
$Albite + 4H^+ + 4H_2O = Al^{3+} + Na^+ + 3H_4SiO_4$	4.14
$C-S-H\ 1.6 + 3.2H^+ = 1.6Ca^{2+} + H_4SiO_4 + 2.18H_2O$	28.00
$C-S-H\ 1.2 + 2.4H^+ = 1.2Ca^{2+} + H_4SiO_4 + 1.26H_2O$	19.30
$C-S-H\ 0.8 + 1.6H^+ = 0.8Ca^{2+} + H_4SiO_4 + 0.34H_2O$	11.05
$Monosulfoaliminate + 12H^+ = 2Al^{3+} + 4Ca^{2+} + SO_4^{2-} + 18H_2O$	73.09
$Ettringite + 12H^+ = 2Al^{3+} + 6Ca^{2+} + 3SO_4^{2-} + 38H_2O$	57.01
$Strätlingite + 10H^+ = 2Al^{3+} + 2Ca^{2+} + H_4SiO_4 + 10.5H_2O$	49.67
$Hydrotalcite + 14H^+ = 2Al^{3+} + 4Mg^{2+} + 17H_2O$	73.76
$Hydrogarnet + 12H^+ = 2Al^{3+} + 3Ca^{2+} + 12H_2O$	49.67
$Brucite + 2H^+ = Mg^{2+} + 2H_2O$	17.11
$Monocarboaluminate + 13H^+ = 2Al^{3+} + 4Ca^{2+} + HCO_3^- + 16.68H_2O$	80.54

III. RESULTS AND DISCUSSIONS

The mix design is used for simulations with 3 natural pozzolan content of 10%, 15% and 20% of weight, the content of cement and lime is fixed 3% and 4%, respectively. The amount of C-S-H and C-A-S-H of the model in two different pozzolan cases is shown in Figure 3.

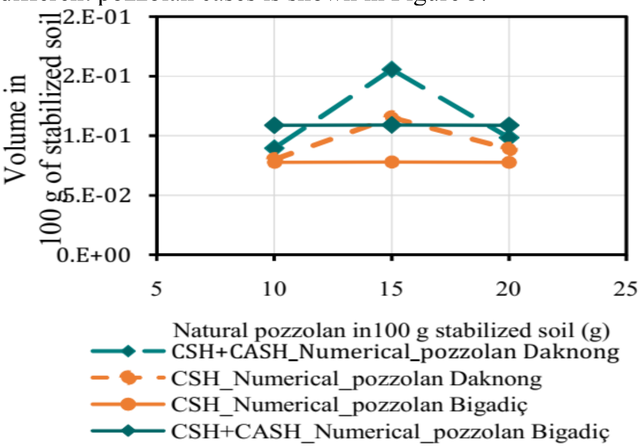

Figure3. Comparison of the mineral content of C-S-H +C-A-S-H in stabilized soil in case of using natural pozzolan extracted in Daknong-Vietnam and Bigadiç, Turkey.

Through figure 3, it is easy to see if with the Daknong natural pozzolan, the mix design soil/pozzolan/cement/lime give optimal mix design with 15% pozzolan used, on the contrary it does not happen with mix design used Bigadiçnatural pozzolan.

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With a content of 10%, 15% and 20% of natural Bigadiç pozzolan used, the mechanical mineral content of C-S-H and C-A-S-H is equivalent, there is no difference between the different content, thus leading to the mechanical strength in these cases is equivalent.

Table 3. Numerical results of the ratio of mineral content of C-S-H and C-A-S-H were formed when using natural pozzolan Bigadiç and Daknong with different amounts.

Content of natural pozzolan used (g/100g đất)	C-S-H Pozzolan Bigadiç/pozzolan Daknong	C-A-S-H Pozzolan Bigadiç/pozzolan Daknong
10	0.97	3.25
15	0.68	0.77
20	0.88	3.25

Table 3 summarizes the difference in the mineral content of C-S-H and C-A-S-H in case of using Bigadiç natural pozzolan on Daknong natural pozzolan.When the natural pozzolan content used is 10%, it can be seen that the amount of C-S-H mineral produced is equivalent regardless of the natural pozzolan, the difference ratio is 0.97. With a 20% content of natural pozzolan,Daknong's natural pozzolan gives greater C-S-H content. However, this difference is smaller than the difference when using 15% of natural pozzolan content, with this content, Daknongpozzolan for the highest C-S-H content and Bigadiç natural pozzolan for constant C-S-H content as analyzed above.

Natural pozzolan Bigadiç produces C-A-S-H content larger, 3 times, when using 10% and 20% natural pozzolan, when compared with the use of Daknong pozzolan. But with the optimal content, Daknong's natural pozzolan produces a higher C-A-S-H content, when the C-A-S-H content ratio in the case of using the Bigadiç/Daknongpozzolan is smaller than 0.77. Natural pozzolan Bigadiç produces larger amounts of C-A-S-H in most of the distribution due to the dissolution of the Clinoptilolite mineral composition, which accounts for large amounts in Bigadiç natural pozzolan, according to the reaction equation (4):

$$\mathbf{Ca_{0.55}Si_{4.9}Al_{1.1}O_{12} \cdot 3.9H_2O + 4.4H^+ + 3.7H_2O = 1.1Al^{3+} + 0.55Ca^{2+} + 2H_2SiO_4} \quad (4)$$

Clinoptilolite is dissolved simultaneously, creating ions Al^{3+}, $Ca2^+$and $H_2SiO_{4(aqueous)}$ dissolved molecules are three simultaneous elements of C-A-S-H, producing many Al^{3+} ions to create a balance for gibbsite $Al(OH)_3$ in the soil is not dissolved as in the case of using Daknong natural pozzolan, because Forsterite and Cristobalite dissolved minerals do not produce Al^{3+} ions causing the system to react unbalanced and dissolve gibbsite $Al(OH)_3$ to produce small amounts of C-A-S-H until the optimal pozzolan content is reached.

The mineral content difference provides mechanical properties for C-S-H + C-A-S-H stabilized soil mix between two types of natural pozzolan depending on the natural pozzolan content used as well as the effect of activated substance content. Used as lime and cement. However, within the limit of the thesis, there is only one content of lime and cement used to understand the activity of natural pozzolan. Based on the comparison of the numerical model with a natural pozzolan exploited in Bigadiç - Turkey, it can be concluded that natural pozzolan extracted in Daknong has a relatively good mineral composition however It is difficult for the process to use because to achieve high-quality quality, the design must be optimized. The optimal content in the case of Daknongpozzolan and not with the Bigadiçpozzolan, is the equilibrium process of a series of reactions presented in Table 2, as well as the equilibrium equation of Clinoptilolite (4). Therefore, the general soil reinforcement mechanism is only relative, in order to better understand the effect of using natural pozzolan to stabilized soil, the thermodynamic model is needed to solve. The equations of reaction sequences take place not merely as single pozzolanic reactions.

IV. CONCLUSIONS

In this paper, geochemical model is proposed to evaluate pozzolanic activity of natural pozzolan. Assessing the performance of Daknong's natural pozzolan, the model shows that this is a relatively good natural pozzolan with up to 24% of the pozzolan content of Forsterite and Cristobalite as compared to the pozzolan itself. Bigadiç - Turkey. However, when using activators such as lime and cement, the design of Daknong's natural pozzolan content is relatively difficult because it is necessary to find the optimal content. The necessity of the thermodynamic model is again confirmed by comparing the activity of natural pozzolan exploited at Daknong - Vietnam and at Bigadiç - Turkey.Due to the limitation of time, many research issues of the stabilized soil mechanism have not been clarified and integrated geochemical model such as the influence of temperature, the effect of pH, the role of cement. in the reaction process with different lime content. At the same time, the time of the reactions from that predicts the development of intensity over time. These issues suggest the future research needs simulation studies combining experiments to improve accuracy and expand the simulation ability of geochemical models in other studies.

REFERENCES

1. B. T. Vu et al., "A Geochemical Model for Analyzing the Mechanism of Stabilized Soil Incorporating Natural Pozzolan, Cement and Lime BT - Proceedings of China-Europe Conference on Geotechnical Engineering," 2018, pp. 852–857.
2. S. Özen, "Pozzolanic activity of natural zeolites: mineralogical, chemical and physical characterization and examination of hydration products," Middle East Technical, 2013.
3. P. Blanc et al., "Thermoddem: A geochemical database focused on low temperature water/rock interactions and waste materials," Appl. Geochemistry, 2012.
4. Van Quan Tran, "Contribution à la compréhension des mécanismes de dépassivation des armatures d'un béton exposé à l'eau de mer : théorie et modélisation thermochimique," Ecole Centrale de Nantes, France, 2016.

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