第十七屆東南亞大地工程研討會

17 SEAGC

The Seventeenth Southeast Asian Geotechnical Conference

May 10~13, 2010, Taipei, Taiwan

Geo-engineering for Natural Hazard Mitigation and Sustainable Development

PROCEEDINGS Vol. I

Theme Sessions

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Organized by

Southeast Asian Geotechnical Society (SEAGS)

Taiwan Geotechnical Society (TGS)

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National Taiwan University (NTU)

Association of Geotechnical Societies in Southeast Asia (AGSSEA)

Modeling of Organic Contaminant Migration through Soil Cement Barrier Using TMVOC

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ABSTRACT: The spill of hydrocarbons from industrial plants is a significant problem that affects ground water. Contaminant migration can widely spread in subsurface by advection and diffusion. The Effect of contaminated ground water becomes more serious if contamination occurs in sandy soil. This paper focuses on the study of LNAPL migration in soil and through a containment barrier. The simulation study of contaminant migration considers 2 scenarios as follows: (1) without groundwater flow and (2) with groundwater flow with a hydraulic gradient of 0.017. The wall, 5 m deep and 1 m thick, was modeled as a containment system. The NAPL spill was modeled with a constant rate release lasting 2 years. The parameters of capillary pressure and relative permeability are considered according to the permeability. The study found that the permeability of soil and the hydraulic gradient of the aquifer were the factors affected the contaminant migration. The results obtained could be used as a guide for the design of impervious wall dimension and properties to properly contain the contaminant migration.

1. INTRODUCTION

Subsurface contamination problems due to the release of toxic substances such as inorganic and organic compounds including hydrocarbon volatile organic compounds (VOCs) may affect the environment and the life cycle of natural animals and humans.
The spill of light non aqueous phase liquid (LNAPL), such as gasoline, into the vadose zone is more risky than the spill of the heavy contaminant (DNAPL) because LNAPL can spread quickly, especially in the presence of high permeability soil. For these reasons, this paper focuses on the benzene (STD) migration behavior through soil cement barrier. The benzene is a aromatic hydrocarbon having a high solubility in water and a non negligible vapor pressure. When spilled into the subsurface it migrates giving rise to multiphase flow processes.

In this study, the simulations took into account different barrier materials and different aquifer hydraulic gradients. The TMVOC simulator was used within the PetraSim 4.2 pre- and post-processing interface. PetraSim is one of the graphical interface available for the TOUGH2 family of reservoir simulators developed at Lawrence Berkeley National Laboratory (USA). TOUGH2 and its derivatives were recognized for their broad range of subsurface simulation capabilities, including heat and multiphase flow and reactive transport.[1,2,3] In the past, modeling of multiphase organic contaminant migration was performed by several authors, such as Abriola and Pinder (1985), Kaluarachchi and Parker (1989), Falta et al.(1995), Soga et al. (2003), Pruess and Battistelli (2003), Fagerlund and Niemi (2003), Dunn (2005), Battistelli (2008).

Soil-cement walls are structures often used to improve the geotechnical properties of soft soil. They can be constructed by 2 methods as follows: (1) rotary mixed method, which is the technique preferred for cohesive soil, with a widespread use in Japan and (2) jet grouting method, which is the technique for both cohesive soil and cohesionless soil. The latter method can especially be used for sandy soil where the injection of cement slurry is more effective than in clay. This approach offers the advantage of building wall columns in both vertical and inclined direction by cement based grout.

2. RESEARCH METHODOLOGY

2.1 Model Characteristics and Material Properties

The conceptual models used in the study are shown in Figure 1. They are two dimensional sections 60.2 m long, 15.1 m thick and 1 m wide. The characteristics of the four models are: (1) no ground water flow (hydraulic gradient equal to zero), (2) ground water flow with a hydraulic gradient of 0.017 (water table difference of 1 m along a distance of 60 m (1/60), (3) no ground water flow with containment (hydraulic gradient equal to zero), and (4) ground water flow with a hydraulic gradient of 0.017 with containment. The spill point of the benzene is located in the unsaturated zone at a distance from left side of 29.6 m for model 1 and 3, and 19.6 m for model 2 and 4. The groundwater table is 2 m below the ground surface for model 1 and 3, while for model 2 and 4, it is 2 m and 3 m deep at the left and right boundaries, respectively. The containment system is 1 m thick, 5 m deep and is located at 1.5 m from the spill point in the left and right direction.

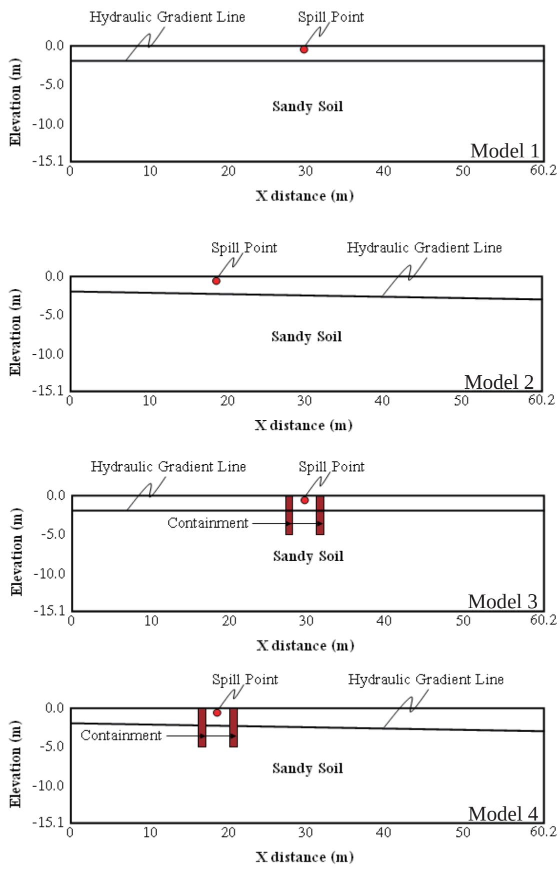


Figure 1 Conceptual models 1, 2, 3 and 4

Effect of intrinsic permeability ($K_i = k_{darcy}\mu/\rho g$) was studied. Three intrinsic permeability values of soil were used which are 10^{-9} m^2, 10^{-10} m^2 and 10^{-11} m^2. The intrinsic permeability of barrier value was also indicated which are 10^{-13} m^2, 10^{-14} m^2 and 10^{-15} m^2. This study considers a total of 24 different cases; basic petrophysical properties are listed in Table 1. The relative permeability and capillary pressure curves for three-phase systems are described according to the Stone (1970) and Parker et al. (1987) models, respectively.[4] The corresponding parameters are summarized in Table 2 and 3 for the relative permeability and the capillary pressure, respectively. The simulations are performed at a constant temperature of 20 °C. The atmospheric boundary conditions are fixed at the grid top and specified as constant absolute pressure of 1.01×10^5 Pa.

Table 1 Main petrophysical properties of rock domains

Soil Criteria	Grain Density	Porosity	Horizontal Permeability		Vertical Permeability	
	kg m^{-3}		m^2	m/s	m^2	m/s
Atmos	2600	0.35	10^{-8}	10^{-1}	10^{-8}	10^{-1}
Soil 1	2600	0.31	10^{-9}	10^{-2}	10^{-9}	10^{-2}
Soil 2	2600	0.35	10^{-10}	10^{-3}	10^{-10}	10^{-3}
Soil 3	2600	0.39	10^{-11}	10^{-4}	10^{-11}	10^{-4}
Wall 1	2600	0.43	10^{-13}	10^{-6}	10^{-13}	10^{-6}
Wall 2	2600	0.47	10^{-14}	10^{-7}	10^{-14}	10^{-7}
Wall 3	2600	0.51	10^{-15}	10^{-8}	10^{-15}	10^{-8}

Table 2 Relative permeability parameters of different rock domains (first Stone's modified model)

Soil criteria	Swr	Snr	Sgr	n exponent
Atmos	0.15	0.05	0.05	3
Soil1,Wall1	0.15	0.05	0.05	3
Soil2, Wall2	0.15	0.05	0.05	3
Soil3, Wall3	0.15	0.05	0.05	3

Remarks: Swr = irreducible aqueous phase saturation, Snr = irreducible NAPL saturation, Sgr = irreducible gas phase saturation, NAPL = non aqueous liquid

Table 3 Capillary pressure parameters of different rock domains (Parker's model)

Soil criteria	Sm	αgn	αnw	n exponent
Atmos	no capillary			
Soil 1	0	100	110	1.84
Soil 2	0	30	33	1.84
Soil 3	0	10	11	1.84
Wall 1	0	1	1.1	1.84
Wall 2	0	3	3.3	1.84
Wall 3	0	0.1	0.11	1.84

Remarks: Sm = limiting saturation, αgn = strength parameter for gas-NAPL, αnw = strength parameter for NAPL-aqueous phase liquid

The applied boundary conditions are shown in Table 4. For this application, the formation of heterogeneities, the seasonal water table fluctuations, and the water infiltration have been neglected.

2.2 Simulated scenarios

The modeling is discretized with 16 layers and 62 columns for a total of 992 elements. The vertical and horizontal spacing is 1x1 m, except the elements of top row which are 1x0.1 m; left and right boundary columns have the spacing of 0.1x1 m. The simulations are divided into several steps as follows: (1) setting up the initial conditions at left and right boundary columns; (2) run to steady state controlled by gravity and capillary forces and subjected to the boundary conditions at lateral and top grid sides specified for each case; and (3) modeling of spill for 2 years starting from the steady state conditions obtained at step 2. The LNAPL spill has been modeled assuming a constant rate of 1.154x10-5 kg/s, equivalent to 1 kg/day. In this study, the effectiveness of barrier is analyzed looking at the effects of aquifer permeability and hydraulic gradient.

Table 4 Boundary conditions applied to simulation

Boundary	Pressure	Condition
Hydraulic Gradient, i = 0		
Top	1.01×10^5	Gas Only
Left (x = 0 m)	1.01×10^5	Gas and Water, Above Water Table (z <= 2.1 m, water sat. = 0.20)
	$1.01 \times 10^5 + 9789z$	Water Only, Below Water Table (z > 2.1 m)
Right (x = 60.2 m)	1.01×10^5	Gas and Water, Above Water Table (z <= 2.1 m)
	$1.01 \times 10^5 + 9789z$	Water Only, Below Water Table (z > 2.1 m)
Boundary	**Pressure**	**Condition**
Hydraulic Gradient, i = 0.017		
Top	1.01×10^5	Gas Only
Left (x = 0 m)	1.01×10^5	Gas and Water, Above Water Table (z <= 2.1 m, water sat. = 0.20)
	$1.01 \times 10^5 + 9789z$	Water Only, Below Water Table (z > 2.1 m)
Right (x = 60.2 m)	1.01×10^5	Gas and Water, Above Water Table (z <= 3.1 m)
	$1.01 \times 10^5 + 9789z$	Water Only, Below Water Table (z > 3.1 m)

3. RESULTS AND DISCUSSION

3.1 Modeling of steady state

The initial conditions to model the spill scenarios were obtained running the system to steady state governed by gravity and capillary forces under the boundary conditions specified for each case. The steady state pore pressure distribution is shown in Figure 2. In case of i = 0, the LNAPL plume spreads symmetrically over the water table, while in the case of aquifer flow, the LNAPL plume moves preferentially following the water table slope.

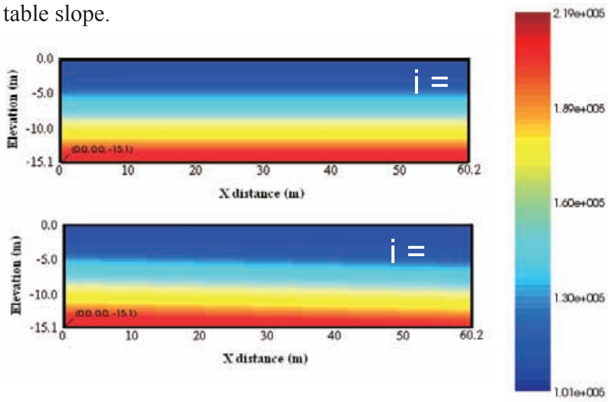


Figure 2 Pore pressure distribution at steady state conditions.

3.2 Migration of LNAPL into subsurface

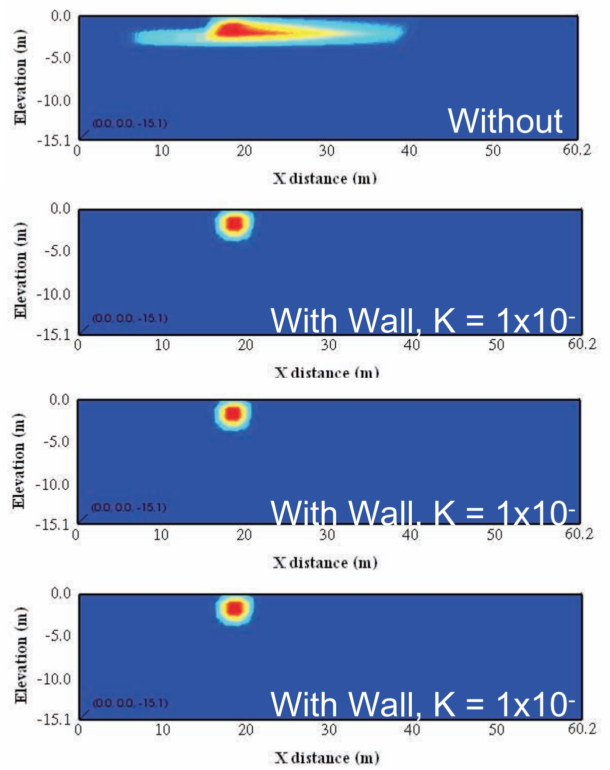
The spill of benzene is modeled at constant rate of 1 kg/day into the vadose zone for 2 years. The simulations are performed under

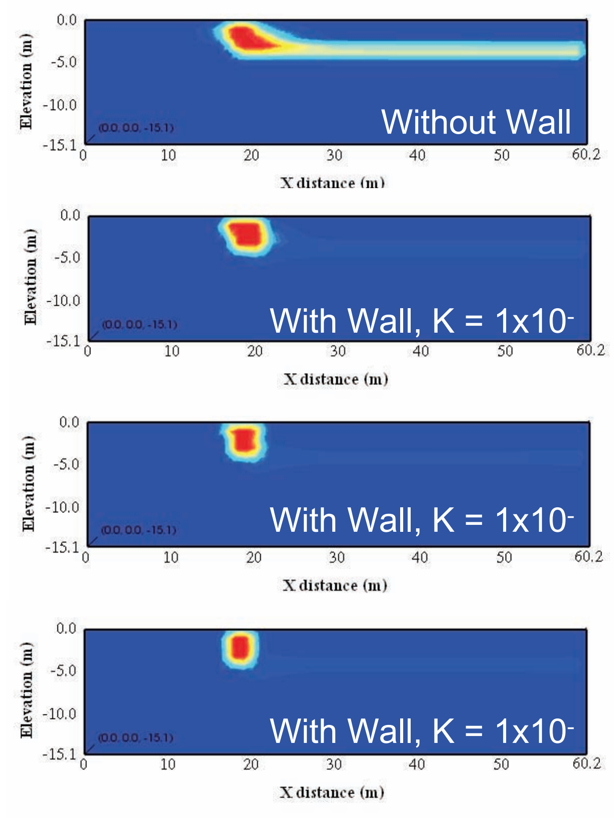
isothermal conditions. In this study, the standard benzene properties (STD) supplied by Petrasim have been used.
The simulation results relative to the total mass fraction of benzene in the aqueous liquid (XVOCW) can be described as follows:

(1) Case i = 0: the benzene moves downward due to gravity (buoyancy) and capillary force; then the LNAPL plume floats on the water table and spreads out laterally because of only capillary force. The depth reached by the dissolved benzene plume below the water table is about 1.5 m and the distance of the benzene migration decreases with the soil permeability. In the presence of containment wall the dissolved benzene is contained by the barrier and can't migrate outside the containment.

(2) Case of i = 0.017: once reached the water table, the LNAPL plume migrates preferentially in the direction of water table gradient. The shape of the dissolved benzene plume changes depending on the permeability and capillary effect. The result of the model scenario without containment shows that if permeability of soil decreases, the LNAPL plume could migrate to longer distances. Higher soil permeability allows a greater evaporation of benzene. Furthermore, a low permeability of the sandy soil has increased the capillary force that it results in a increase in lateral movement of contaminated plume. Because the capillary force between LNAPL (wetting) and air (non wetting) is larger in the finer soil. The results of the model scenario with wall containment show that the benzene migration is reduced by the containment. The dissolved benzene plume moves downward along the barrier and some benzene can flows under the wall base when the soil has lower permeability as shown in Figure 3.

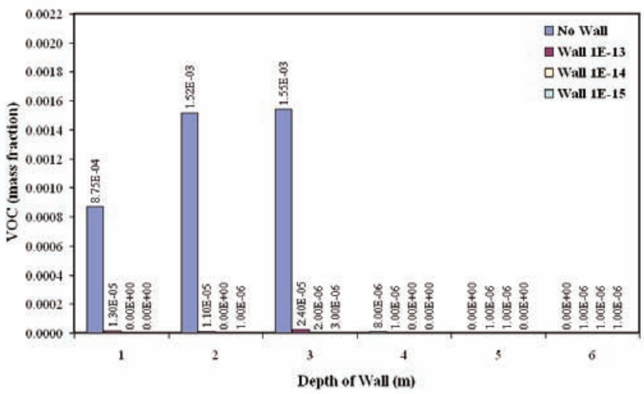
The total mass fraction of VOCs dissolved in the aqueous phase outside the containment zone at depth of 1 – 6 m below the ground surface in the case of i = 0 with containment is reduced close to zero, as shown in Figure 4a – 4c. For the case of i = 0.017, the concentration of the benzene increases at the end of the barrier according to permeability decrease due to the effect of the ground water flow as shown in Figure 4d – 4f. They can be shown that the barrier is able to stop or reduce the overall contaminant flux to contaminated area.



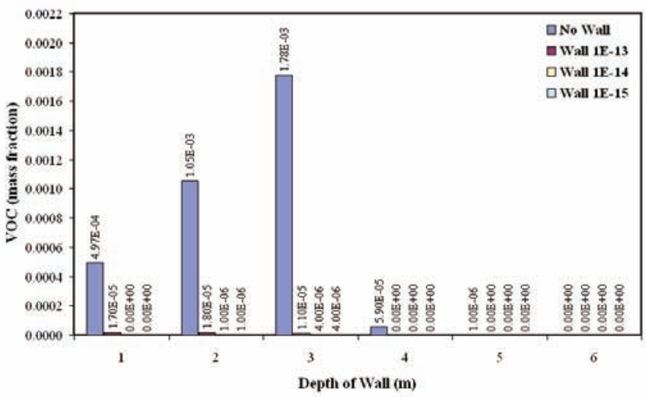


(b) Intrinsic Permeability of Soil, K = $1x10^{-11}$ m^2

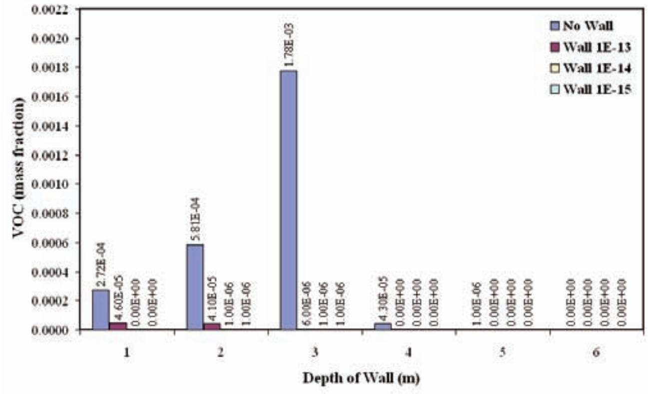
Figure 3 Plume of dissolved VOCs mass fraction after 2 years of spill in sandy soil with hydraulic gradient, i = 0.017.



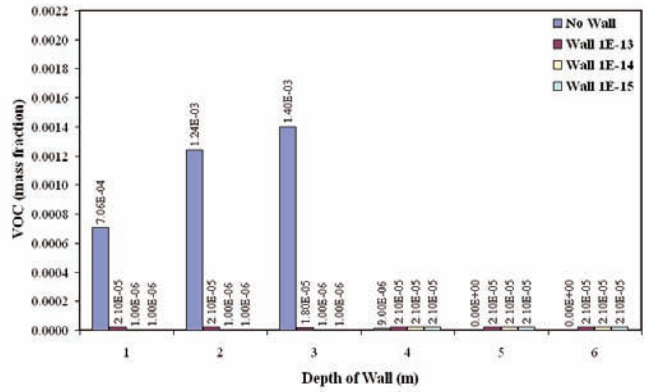
(a) K = $1x10^{-9}$ m^2 and i = 0



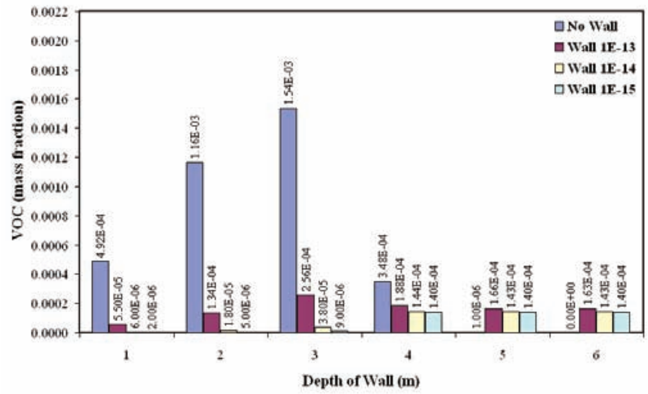
(b) K = 1x10^{-10} m^2 and i = 0



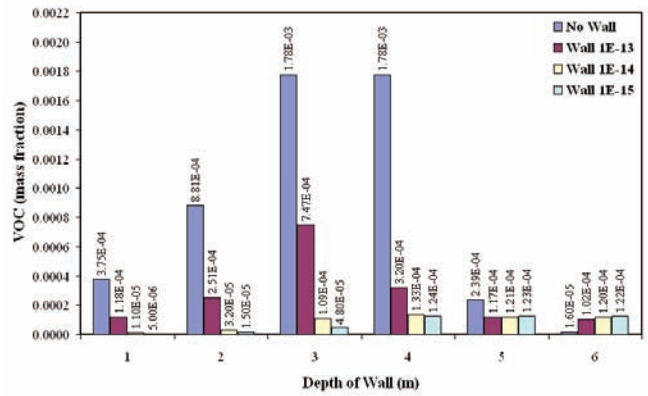
(c) K = 1x10^{-11} m^2 and i = 0



(d) K = 1x10^{-9} m^2 and i = 0.017



(e) K = 1x10^{-10} m^2 and i = 0.017



(f) K = 1x10^{-11} m^2 and i = 0.017

Figure 4 Mass fraction profile of dissolved VOCs after 2 years

of spill along to outside the wall.

4. CONCLUSIONS

This paper presents simulation of benzene migration in the subsurface as a consequence of a constant rate spill in the unsaturated zone. Several scenarios have been modeled with a phreatic aquifer in a sandy soil of varying permeability, with different hydraulic gradients and with or without the presence of a vertical containment wall. Simulations results reveal that the soil-cement barrier can reduce the contamination of the benzene and show that soil permeability and water table hydraulic gradient are the significant factors.

The benzene migration in the case of i = 0, only occurs by gravity driven NAPL plume flow and diffusion of dissolved benzene in the groundwater. In the presence of aquifer flow, dissolved benzene may be transported over long distances by advective flow. Without the groundwater flow, the contaminant migration is contained by the soil-cement barrier in the vadose zone; the dissolved benzene plume reaches less than 2 m below the water table. Consequently, the depth of the soil-cement wall should be more than 2 m below the ground water level. With ground water flow, the concentration of contamination depends on the hydraulic gradient which enhances the transport processes. The hydraulic gradient has an impact on the depth of contaminant migration outside the wall. From the scenarios simulated, it can be concluded that soil-cement barriers can be used to limit the spread of benzene spilled in the unsaturated zone. Modeling studies such as that described may help in the design of containment operations and in risk assessment studies.

That presented is a preliminary study dealing with the processes controlling the migration of VOCs spilled in the vadose zone in the presence of vertical containment walls in sandy aquifers. The properties of the soil-cement used in these simulations are derived from bibliographic sources. Experimental derived properties will be considered in future simulation works.

5. ACKNOWLEDGMENT

I would like to thank the Office of the Higher Education Commission, Thailand for supporting by grant fund under the program Strategic Scholarships for Frontier Research Network for the Join Ph.D. Program Thai Doctoral degree for this research and also thank Rajamangala University of Technology Rattanakosin for providing funding for this research. Furthermore, thanks are due to Alfredo Battistelli for information about the TMVOC simulator and for valuable suggestions.

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Using Circulating Groundwater as Cooling Medium for Air Conditioner at NTUST

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ABSTRACT: To reduce the heat-island effect in urban area, this paper reports the preliminary results of a newly developed circulation groundwater system used for cooling air conditioner. The circulating groundwater is from the underground reservoir in Chingmei stratum which is located about 50m below Taipei city. To obtain the actual operation data of this circulating well system, it was connected to an air conditioner in a newly constructed building at NTUST campus. According to the measured temperature of the groundwater, it varies from 24℃ (winter) to 26 ℃ (summer). The transmissivity of Chingmei stratum is estimated to be 0.049 m^2/min (at the upper layer) to 0.181 m^2/min (at the lower layer) by pumping test. A 15RT package air-conditioner was operating continuously in summer and winter time. The thermal and hydraulic responses of the Chingmei stratum were recorded. This system consists of only a water pump and a plate type heat-exchanger. It is very compact in size. It can not only save up to 95% in space but also save energy. It generates no heat exhaust to the air and consumes no water. Lastly and very importantly, it is very quiet and clean to operate.

1. INTRODUCTION

Global warming and urban heat-island effect are the deeply concerned issues worldwide. This phenomenon is especially significant in Taipei city due to its basin topography. The heat exhausted to air from cooling towers of air-conditioner is driving temperature up in recently years. However, air-conditioner system is a must in the summer time for most of the cities to cool down indoor temperature. Warming climate will push people to use more air-conditioners. In addition to temperature problem, cooling tower tends to result in Legionella Pneumophila problem [1] and also makes noise to the neighbourhood. To eliminate the problems associated with the cooling tower, an alternative system that adopts the circulating groundwater as the cooling medium for air-conditioner is proposed.

As estimated, there is about 68.4 billion m^3 [2] of groundwater stored in the Chingmei gravel stratum underlying Taipei basin. The temperature of groundwater in this stratum ranges from 24 to 28℃[3]. Potentially, it can be a big resource for the cooling need of air-conditioners. But no pumping without permission is allowed in Taipei city to prevent any pumping induced ground settlement. Therefore, the groundwater being pumped out is required to recharge back to the aquifer in Chingmei gravel stratum after cooling down the air-conditioner (see Figure 1). Similar idea was also reported such as the Aquifer Thermal Energy Storage (ATES) and the Geo-thermal pump or Heat pump. The underground thermal energy storage (UTES) concept is based on the principle of using the earth to store heat (or cold) for later use. ATES is a subset of underground thermal energy storage (UTES) technology. However, both systems are more often used in high latitude countries where the use of underground thermal energy is very different from countries in tropical or subtropical regions. For example, the normal summer temperature in Taipei can easily go beyond 30℃ and using air-conditioner to cool down the indoor temperature is inevitable. To adsorb massive heat generated from air-conditioner in short time, it can not be done by the earth alone as proposed by ATES method. Therefore, we need groundwater to take part in this heat exchange process and helps to adsorb and carry away the heat exhausted from the air-conditioner.

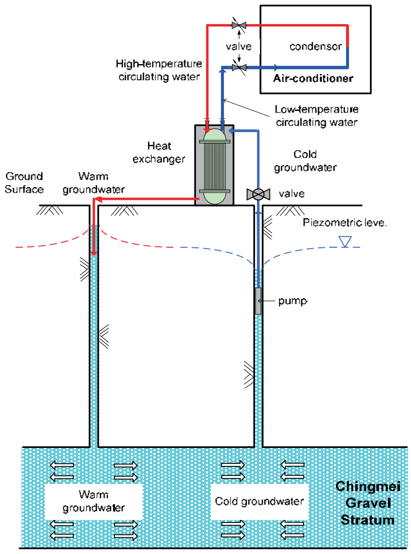

Figure 1 Schematic diagram of circulating groundwater system (pumping/recharging well placed separately, circulating via the same layer and aquifer)

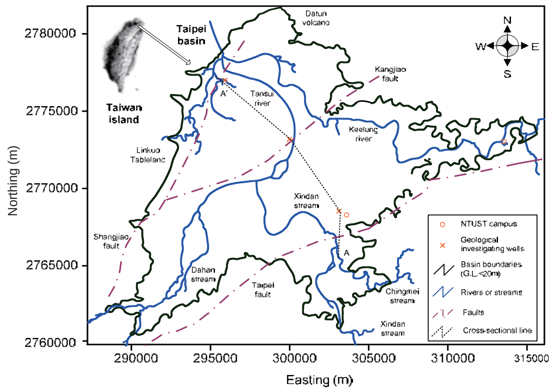

Figure 2 Geographical structures of Taipei basin, observation wells locations, and test site location

2. HYDROGEOLOGY OF TAIPEI BASIN

Taipei Basin (Figure 2) which is located in the northern Taiwan covers approximately an area of 243 km^2 with the average elevation about 20m above sea level. Taipei Basin is surrounded by Datun volcanoes in the north; by Linkou tableland in the west; and by hills and mountains in the east and the south. Several major rivers meander through the Taipei basin, namely Tanshui river, Keelung river, Xindian river and Dahan river. Sediments deposited from different rivers vary from one to another. Generally, soft clays were deposited from Keelung river; gravels were deposited from Xindian river; and sandy layers were deposited from Dahan river. Basically, the sandy and clayey deposits are underlain by the gravel deposit in Taipei basin.

2.1 Stratigraphy

Based on the boring log data gathered from the basin, a schematic diagram of the basin profile can be drawn in Figure 3. Shungshan

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