Uva Wellassa University, Sri Lanka
End Semester Examination – February/March 2012

MRT 454-2 Computers in Groundwater Modeling

Duration: Two (02) hours

Uva Wellassa University

Total four (04) questions
Answer **all** questions
Computer facility will be provided
Use PHREEQC Interactive (Version 2) computer program to answer Question 04 (ii) and 04 (iii). You are allowed to use PHREEQC User's Guide.

Part – A

01. Consider the stream function u satisfying the Poisson's equation,

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=9 \;\; ; \; 0 \le x \, , \, y \le 1$$

with following boundary conditions

$u=1 \quad on \quad 0 \le x \le 1 \, , \, y=1$

$\frac{\partial u}{\partial y}=0 \; ; \quad 0 \le x \le 1 \, , \, y=0$

$u=0 \quad$ *elsewhere on the boundary.*

i. Classify the above equation.

ii. By taking an equal grid size of $\frac{1}{3}$ along both directions write down the finite difference scheme.

(25 marks)

02. i. Derive the key steps of the Crank Nicolson scheme to estimate an approximate solution to the following equation.

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2} \;\; ; \; 0 \le x \le 1 \, , \, t > 0$$

ii. Applying the answer of Section I, use the Crank Nicolson scheme to find an approximate solution to the equation subjected to following boundary value and initial conditions

$$u(0,t) = 0 \ , \ u(1,t) = t \quad for \ \ t > 0$$

$$u(x,o) = \begin{cases} 2x & ; \ 0 \le x \le 1/2 \\ 2 & ; \ 1/2 < x \le 1 \end{cases}$$

with the time step $k = \frac{1}{8}$ and mesh size $h = \frac{1}{4}$ for two time-steps.

(25 marks)

Part – B

03. i. The solubility constant of the fluorite (CaF_2) dissolution reaction at 25 ^{0}C is $10^{-10.57}$. Write an expression for logK.

ii. A groundwater sample contains 0.249 mmol/l Ca^{2+} and 0.289 mmol/l F^-.

(a) Comment on the saturation state value with respect to fluorite.

(b) Will fluorite precipitate out from this water sample? Explain why.

iii. What would happen if gypsum ($CaSO_4.2H_2O$) is added to the above water sample?

iv. Sketch the variation of [Ca^{2+}] on a graph of [F^-] vs [Ca^{2+}] when gypsum is added.

(20 marks)

04. i. Following table gives the analytical results of groundwater samples collected from two geologic units. Comment on the lithology of these units based on water composition.

Parameter	Unit A	Unit B
	Conc. (mmol/l)	Conc. (mmol/l)
Na^+	0.18	0.19
K^+	0.01	0.01
Ca^{2+}	0.15	2.30
Mg^{2+}	0.30	0.11
Cl^-	0.38	0.41
HCO_3^- (as alkalinity)	0.47	4.34
SO_4^{2-}	0.12	0.14
pH	6.83	7.17

Use PHREEQC Interactive (Version 2) computer program to answer following questions. [Accept default values for any undefined parameter]

ii. Make an input file with above solutions and execute the program.

(a) Write down the calculated ionic strengths of the two solutions.

(b) Describe your observations regarding saturation states of solid phases in the above two systems.

iii.(a) Suppose that the two geologic units have lateral continuity and groundwater from Unit A starts to flow into B. The two solutions mix with each other resulting in a new composition.

Find out the new composition of the solution [*Hint: Use **MIX** keyword*]. Discuss your observations on the changes taking place in the solution composition.

(b) Give your observations on mineral dissolution/precipitation in the system.

(c) Calculate the number of moles of calcite that should be introduced into Unit B if the new system is to be saturated with respect to calcite. [*Hints: Use the solution "Mix 1" of above mixing with **USE** keyword; Introduce calcite with **EQUILIBRIUM PHASES** keyword; Consider saturation indices*]
(Ca 40.07, C 12.01, O 15.99)

(30 marks)