Contaminant Transport with Groundwater Flow in Unconfined Aquifer (Two-dimensional Numerical Solution)

DWI TJAHJANTO and AMIR HASHIM MOHD KASSIM
Department of Water Resources and Environmental Engineering
University College of Technology Tun Hussein Onn (KUiTTHO)
86400 Parit Raja, Batu Pahat, Johor
MALAYSIA

Abstract: - The nature of physical process of groundwater contamination transport generates complexity in the theoretical formulation. The governing equations, which are 2nd order PDE (partial differential equation), are solved numerically using a finite difference method. To perform the numerical equations, computer code has been written in MATLAB, and a program has been developed. The aquifer is idealized as an unconfined aquifer system including the well in which the solution domain is stated to be two-dimensional. This method has yielded the relationship between contaminant concentration distribution and time in the aquifer.

Key-Words: - Numerical Solution - Unconfined Aquifer - Contaminant Transport

1 Introduction

De Jong (1958), Wilson and Miller (1978) and Bedient et al. (1994) formulated and solved the transport of contaminant in unconfined aquifer analytically with the help of Laplace and Hansel transformation technique. Their finding is applicable but not handy, especially in the using of values of erfc and Bessel function. Some researchers such as Smith and Schwartz (1980), Hwang, et al. (1985), Frind and Matanga (1985), Daus and Frind (1985), Burnett and Frind (1987), Dillon (1989), Lindstrom and Boersma (1989), Leij and Dane (1990) and many other researchers have proposed a good method to solve the problem of contaminant transport by either analytical or numerical solution.

However, they do not consider the dispersion spreading in the vertical direction where y-axis is the vertical direction and x-axis is the horizontal direction of the aquifer domain and the source of contaminant is injected from a certain point of the upper domain of aquifer. Hence, this study is to describe the transport of pollutant (chloride) with groundwater flow in unconfined aquifer where the aquifer domain is bounded by a well in the right side and recharged by chloride in the upper left side (Fig.1).

2 Problem Formulation

Equation below is taken as the governing equation of pollutant transport for the case of non-reactive tracer in two-dimensional of x and y direction in the aquifer system.

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} - \frac{C_0 W^*}{nb} \quad (1)$$

Where C is solute concentration, C_0 is solute concentration in a fluid source or sink, t is time, D_x and D_y are coefficient of hydrodynamic dispersion, v_x and v_y are pore water velocity, n is porosity of aquifer, b is saturated thickness of aquifer. W* is source or sink term (Javandel, 1984 and Bedient, 1994).

3 Problem Solution

Equation (1) is then approximated by spatial discretisation using finite difference formula. If the domain of equation is (x,y) = (0,P), (0,L) and the width of each discretisation of grid is h = P/N and k = L/M, then the formula is expressed as (Anderson, 1984).

$$\left(\frac{\partial^2 C}{\partial x^2}\right)_{i,j} = \frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{h^2} \quad (2)$$

$$\left(\frac{\partial^2 C}{\partial y^2}\right)_{i,j} = \frac{C_{i,j+1} - 2C_{i,j} + C_{i,j-1}}{k^2} \tag{3}$$

$$\left(\frac{\partial C}{\partial x}\right)_{i,j} = \frac{C_{i+1,j} - C_{i-1,j}}{2h} \tag{4}$$

$$\left(\frac{\partial C}{\partial y}\right)_{i,j} = \frac{C_{i,j+1} - C_{i,j-1}}{2k} \tag{5}$$

Substitution of equations (2), (3), (4) and (5) to equation (1) produces:

$$\begin{aligned}\left(\frac{\partial C}{\partial t}\right)_{i,j} &= \left(\frac{D_x}{h^2}\right)C_{i-1,j} - \left(\frac{D_x}{h^2}\right)C_{i,j} + \\ &\left(\frac{D_x}{h^2}\right)C_{i+1,j} + \left(\frac{D_y}{k^2}\right)C_{i,j} - \left(\frac{D_y}{k^2}\right)C_{i,j-1}\end{aligned} \tag{6}$$

New parameters such as α, β, γ, δ, ε and η are introduced as follows:

$$\begin{aligned}&\alpha = \left(\frac{D_x}{h^2} + \frac{V_x}{2h}\right), \beta = \left(\frac{D_y}{k^2} + \frac{V_y}{2k}\right), \\ &\gamma = \left(\frac{2D_x}{h^2} - \frac{2D_y}{k^2}\right), \delta = \left(\frac{D_x}{h^2} - \frac{V_x}{2h}\right), \\ &\varepsilon = \left(\frac{D_y}{k^2} - \frac{V_y}{2k}\right), \eta = -\frac{C_0 W^*}{nb}\end{aligned} \tag{7}$$

Then equation (7) becomes:

$$\begin{aligned}\left(\frac{\partial C}{\partial t}\right)_{i,j} &= \alpha C_{i-1,j} + \beta C_{i,j-1} + \gamma C_{i,j} + \\ &\varepsilon C_{i,j+1} + \delta C_{i+1,j} + \eta\end{aligned} \tag{8}$$

The boundary conditions are stated as (Brown, 1986):

$$\begin{aligned}&C(x = 0, y, t) = 0, \\ &C(x = L, y, t) = -\alpha C_0^{-2y} \\ &\left(\frac{\partial C}{\partial y}\right)_{i,1} = 0, \text{found} : C_{i,0} = C_{i,2}, \text{for all } i \\ &\left(\frac{\partial C}{\partial y}\right)_{i,M} = 0, \\ &\text{found} : C_{i,M+1} = C_{i,M-1}, \text{for all } i\end{aligned} \tag{9}$$

According to equation (8), for the index value of i = j = 1, then equation (8) becomes:

$$\left(\frac{dC}{dt}\right)_{1,1} = \gamma C_{1,1} + (\beta + \varepsilon)C_{1,2} + \delta C_{2,1} + \eta \tag{10}$$

Furthermore, the boundary condition is stated as:

$$C_{0,1} = 0;\ C_{1,0} = C_{1,2} \tag{11}$$

And then equation (10) becomes:

$$\left(\frac{dC}{dt}\right)_{1,1} = \gamma C_{1,1} + (\beta + \varepsilon)C_{1,2} + \delta C_{2,1} + \eta \tag{12}$$

Using the above boundary conditions, then equation (12) is written as follows:

$$\begin{bmatrix} \lambda & \beta+\varepsilon & & \delta & & & & & \\ \beta & \lambda & \beta & & \delta & & & & \\ & \beta+\varepsilon & \gamma & & & \delta & & & \\ \alpha & & & \gamma & \beta+\varepsilon & & \delta & & \\ & \alpha & & \beta & \gamma & \beta & & \delta & \\ & & \alpha & & \beta+\varepsilon & \gamma & & & \delta \\ & & & \alpha & & & \gamma & \beta+\varepsilon & \\ & & & & \alpha & & \beta & \gamma & \beta \\ & & & & & \alpha & & \beta+\varepsilon & \gamma \end{bmatrix}$$

$$\begin{bmatrix} C_{11} \\ C_{12} \\ C_{13} \\ C_{21} \\ C_{22} \\ C_{23} \\ C_{31} \\ C_{32} \\ C_{33} \end{bmatrix} + \begin{bmatrix} \alpha C_0 e^{-2} \\ \alpha C_0 e^{-4} \\ \alpha C_0 e^{-6} \\ \eta \\ \eta \\ \eta \\ \eta \\ \eta \\ \eta \end{bmatrix} = \frac{dC}{dt} \tag{13}$$

While the initial value is stated as:

C(i ≥ 0, t = 0) = 0

Equation (13) with its initial condition is an initial value problem of a system of ordinary differential equation and the general form is:

$$C' = f(t, C), \quad C(t,0) = C_0, \quad C, f \in R^N \tag{14}$$

Due to equation (12) has a constant coefficient, then the equation is written as follows:

$$A\,C = B \tag{15}$$

The sixth order implicit Runge-Kutta is the method used for solving the initial value problem.

This method is expressed in the table of Butcher as follows (Gear, 1971).

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & & a_{1s} \\ c_2 & a_{21} & a_{22} & & a_{2s} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_s & a_{s1} & a_{s2} & & a_{ss} \\ \hline & b_1 & b_1 & & b_s \end{array} \tag{16a}$$

where:

$$k_i = f'\left(t_{n-1} + \delta C_i, C_{n-1} + \delta \sum_{j=1}^{s} a_{ij} k_j \right) \tag{16b}$$

$$C_n = C_{n-1} + \delta \sum_{i=1}^{s} b_j k_i \tag{16c}$$

In equation (16), C_n is the solution vector of (n) step, δ is the step-size of each step, and C_{n-1} is the solution vector of the previous step.

Kuntzmann-Butcher formula is a form based on the sixth order implicit Runge-Kutta (Hairer, et al., 1987) as follows:

$$\begin{array}{c|ccc} \frac{1}{2} - \frac{p}{10} & \frac{5}{36} & \frac{2}{9} - \frac{p}{15} & \frac{5}{36} - \frac{p}{30} \\ \frac{1}{2} & \frac{5}{36} - \frac{p}{24} & \frac{2}{9} & \frac{5}{36} - \frac{p}{24} \\ \frac{1}{2} + \frac{p}{10} & \frac{5}{36} - \frac{p}{30} & \frac{2}{9} - \frac{p}{15} & \frac{5}{36} \\ \hline & \frac{5}{18} & \frac{4}{9} & \frac{5}{18} \end{array} \tag{17}$$

where: $p = \sqrt{15}$

The application of equation (16) on equation (15) yields linear equation in (k) as follows.

$$\begin{bmatrix} i - a_{11}dA & -a_{12}dA & \cdots & -a_{1s}dA \\ -a_{21}dA & -a_{22}dA & \cdots & -a_{2s}dA \\ \vdots & \vdots & \ddots & \vdots \\ -a_{s1}dA & -a_{s2}dA & \cdots & -a_{ss}dA \end{bmatrix} \begin{bmatrix} k_1 \\ k_2 \\ \vdots \\ k_{ss} \end{bmatrix} = \begin{bmatrix} B \\ B \\ \vdots \\ B \end{bmatrix} \tag{18}$$

Automaticly, after equation (18) is solved, then the solution of $C_n(t = t_n)$ is calculated based on the previous value of (C_{n-1}), which is as follows.

$$C_n = C_{n-1} + \delta b_1 k_1 + \delta b_2 k_2 + ... + \delta b_s k_s \tag{19}$$

Equation (19) is obtained adaptively on the value of δ. The adaptive process is explained through the following algorithm.

Adaptive Algorithm

Input: δ_{01}, C_0, t_0, t_f

Ouput: C_f

$t_n = t_0$

While $t_n < t_f$

(1) $\delta_1 = \delta_0$, solve equation (17) and (18) with $\delta = \delta_1 \rightarrow$ obtained C_1

(2) $\delta_2 = \frac{1}{2}\delta_1$, solve equations (17) and (18) with $\delta = \delta_2$

(3) $\delta_2 = \frac{1}{2}\delta_1$

(4) if $|C_1 - C_2| > \varepsilon$ then $\delta_0 = \frac{1}{2}\delta_1$, go to (1)

(5) $t_n = t_{n+}\delta_1$

End

4 Results and Discussion

The alteration of contaminant concentration towards radius of well obtained from both, laboratory experiment of sand tank model and numerical solution is plotted in Fig.3. It does not indicate a good agreement between them. Curves of laboratory data have a tendency to be steeper than curves of numerical solution. At zero cm of x, the deviation of curves is not significant. But when the values of x are in the range of 40 to 80 cm, the deviation becomes greater. Curves of laboratory data tend drop after a distance of 40 cm until 80 cm. This is maybe the layer of aquifer is not perfectly uniform. The placement of sand in the physical model may not cause uniformity in whole layer of the aquifer. Weight of the upper layer could press the lower layer to cause changes of either porosity or hydraulic conductivity to become smaller. Also during the collection of data, footstep of observers on the top layer could cause changes of uniformity of the layer of aquifer.

However, after changing $D_y = 0.1\ D_x$, then a better result is gained as shown in Fig.4. Previous researchers such as Tang and Aral (1992) assumed the value of D_y to be ten percent of D_x as well.

The numerical solution is also applied for a big scale field problem as follows: An underground tank leaches a liquid waste of chloride into an unconfined aquifer having a hydraulic conductivity of 2.15 m/day, an effective porosity of 0.1, a hydraulic gradient of 0.04 m/m, an initial concentration of 1000 mg/L and longitudinal dispersivity of 7.5 m. The question is how long the time taken for the contaminant concentration to reach 100 mg/L at distance L = 750 m by neglecting any degradation processes. The time given by analytical solution (Bedient at al., 1994) to reach the contaminant concentration for C = 100 mg/L and at distance L = 750 m is after 25.88 months. While, the numerical solution yielded results as plotted in Fig.2 reaches for C = 100 mg/L after 30 months. Both results have a bit difference; however, it needs to compare with monitoring field data.

5 Conclusions

- The problem of contaminant transport in unconfined aquifer has been formulated and solved with the help of numerical technique.
- A type of computer program written in MATLAB has been developed which can be employed to analyze the contaminant transport in unconfined aquifer system.
- Two-dimensional solution is much better solved numerically as the solution enables the representation of the actual field problem by using complex boundary system.
- Results of the contaminant transport example show the behavior of the spreading of contaminant where the dominant seepage velocity effects in a contaminant concentration situation.

References:

[1] Abdul Khader, M.H., Mohd. Kassim, A.M., and Tjahjanto, D. (1996). An Analytical Solution of Groundwater Contamination Transport in Multi-layer Aquifer. *Proc. 10th Congress of the Asian Pacific Division of the International Association for Hydraulic Research*, vol.2, 583-590.

[2] Anderson, D.A., Tannehil, J.C., and Pletcher, R.H. (1984). Computational Fluid Mechanics and Head Transport. *Hemisphere Publ. Corp., New York*.

[3] Anderson, M.P., and Woessner, W.W. (1992). Applied Groundwater Modeling. *Academic Press, San Diego, California.*

[4] Bedient, P.B., Rifai, H.S., and Newell C.J. (1994). Groundwater Contamination. PTR Prentice-Hall, *Englewood Cliffs, New Jersey.*

[5] Gear, W.C. (1971). Numerical Initial Value Problem in Ordinary Differential Equations. *Prentice-Hall Inc. New Jersey.*

[6] Gorelick, S.M. (1984). A Model for Managing Sources of Groundwater Pollution. *J. Water Resources Res*. 18(4), 773-781.

[7] Hairer, E., Noorsett, S.P., and Wanner, G. (1987). Solving Ordinary Differential Equation 1, Non Stiff Problem. *Springer-Verlag, Berlin.*

[8] Javandel, L., Doughty, C., and Tsang, C.F. (1984). Groundwater Transport Handbook of Mathematical Models. *American Geophysical Union, Water Resources Monograph 10, Washington, DC.*

[9] Tang, Y., and Aral, M.M. (1992). Contaminant Transport in Layered Porous Media 2. *Applications. J. Water Resources Res.* 28(5): 1399-1406.

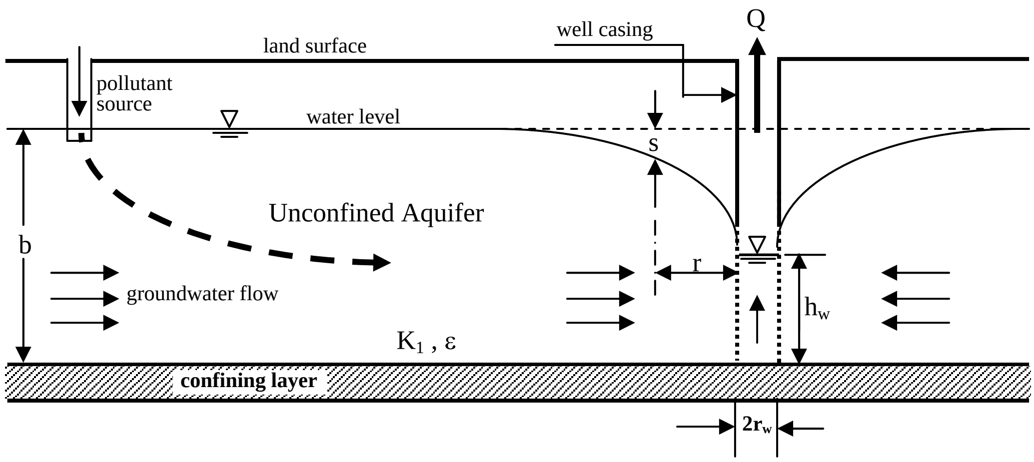

Fig.1: Definition Sketch of Contaminant Transport with Groundwater Flow

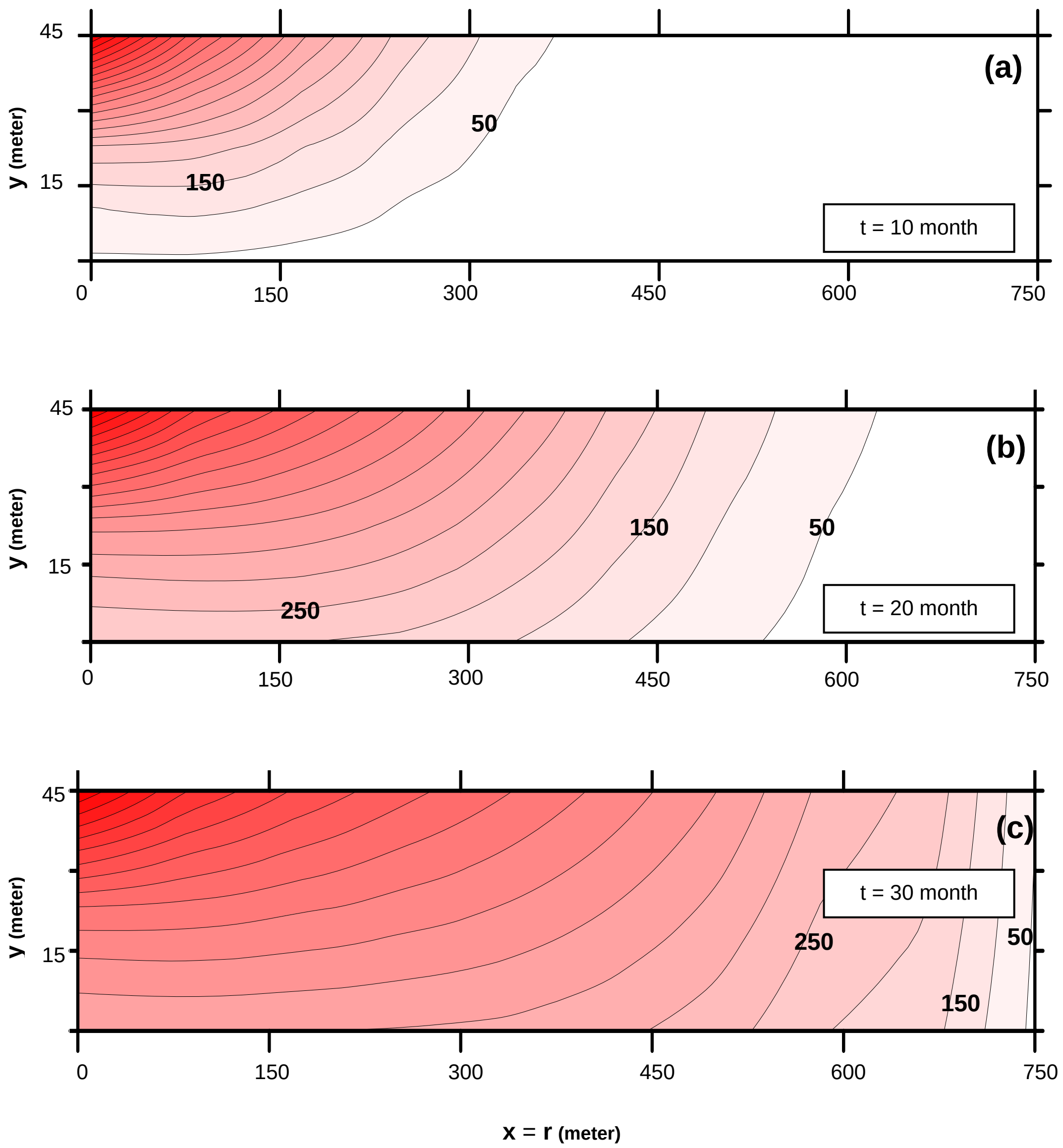

Fig.2: Distribution of contamination concentration in the domain of unconfined aquifer as results of running the program where H_1=45m, h_w=15m, C_0=1000mg/L, n=0.01 and α=7.5m

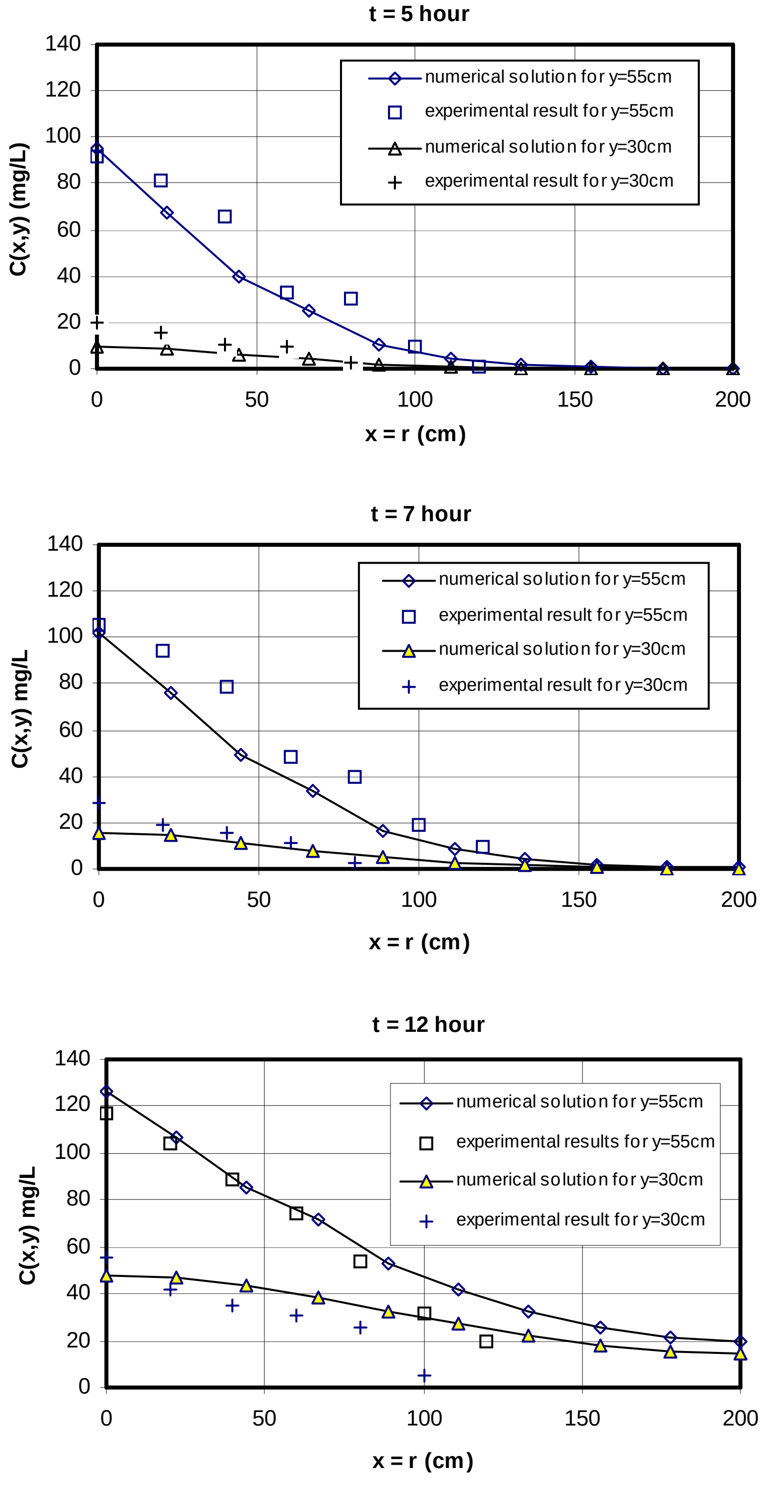

Fig. 3: Change of contaminant concentration towards radius of well for H_1=60cm, h_w=15cm, n=0.363, and C_0=200mg/L, comparison between results of numerical solution and laboratory experiments.