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SIMULATION OF DIFFUSION PHENOMENA OF CHLORINE ION THROUGH SOIL USING CELLULAR AUTOMATON METHOD

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Abstract: In this study, we propose a simulation model for chlorine-ion diffusion using cellular automaton (CA), where mobile-water and immobile-water are postulated to exist in soil. Simulation results obtained from this proposed model are compared with those of observation by column experiment to verify the applicability of the model for soil pollution phenomena. The model could be reproduced tailing phenomena in breakthrough curves, and estimated distribution of immobile water in the soil column. It is shown that the complexity phenomena such as diffusion of soil pollution can be simulated simply and precisely by CA model more simply than numerical analysis.

Keywords : cellular automaton, diffusion phenomena, chlorine ion, immobile-water

1. Introduction

Soil and ground water contamination has been spread due to the utilization and effluent of harmful materials from industrial factories or the illegal dump of poisonous gas weapon. By recent land development works for housing and city-reconstruction, the soil contamination is actualized, proposing it as a social problem. The law to prevent the soil contamination has been enforced from March, 2003 to promote the legal countermeasures against the soil contamination in Japan. Correct conjecture of soil contamination was required before the cleaning-up or the restoration of contaminated soil. The boring research was sometime done, but the accurate grasp was hard because of economic reason. It was general that information was multiplied by the numerical analysis of equations to govern the soil contamination. Then, the numerical analysis was paid much attentions to develop[1),2),3),4)].

However, when natural phenomenon was estimated using the numerical analysis to obtain highly accurate results, more complicated equations related to the phenomenon should be composed and solved. Moreover, the initial and boundary conditions should be established more sophisticatedly, otherwise simple conditions sometime led large errors. Actually, it was very hard to elucidate the phenomenon of contaminated materials in a complicated ground circumstances. For example, whole situation of the arsenic contamination at Kamisu-shi, Ibaraki, Japan, which appeared 2002 fiscal year, was not grasped until the present time, though the boring research was carried out.

In the present study, cellular automaton method (CA), which was one sort of computer program, was applied to develop the simulation system for diffusion of soil-contaminated materials. Applying the CA to the diffusion simulation of soil-contaminated materials, it was expected to calculate rather simply the complicated phenomena by means of no construction of the governing equations and smaller parameters. As first attempt to develop the calculation system, diffusion simulating model for chloride ions, which was able to hold rather stable condition, was investigated to verify the applicability of the CA to the simulation of soil-contamination.

2. CA

(1) Characteristics of CA

The CA method was devised by Johan von Neuman and Stanislow Ulam at 1948 and was firstly opened on

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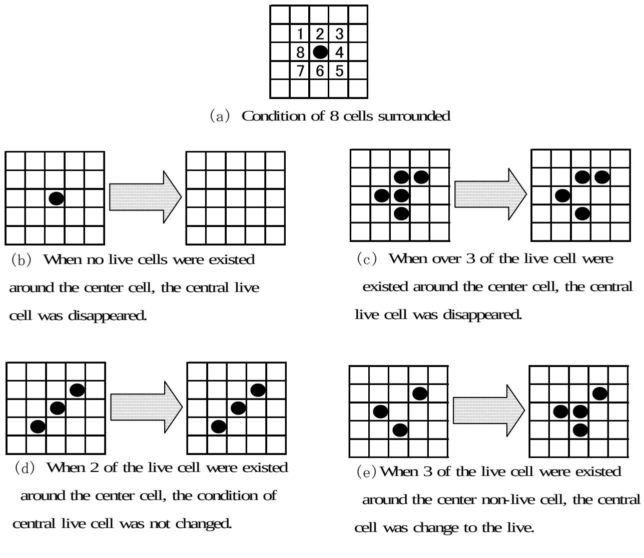
Hikson symposium regarding to brain mechanism for action. The objective space was divided to cells and condition variables, which were defined by dispersed numbers for each cell, were varied timely applying the local rule which worked only between near cells [5),6)]. By accumulation of local interaction, the whole structure was spontaneously formed, which was characteristic of the CA.

The conventional method to realize complicated phenomena such as differential equation model was called as a top-down method and from the differential equations at the top, the characteristic phenomena was obtained deductively by numerical analysis such as the calculus of finite differences. In the other hand, the method using self-organization such as the CA was called a bottom-up method. The characteristic of CA was not only to substitute the differential equations but also to express the irregular phenomena.

(2) Life game

As two-dimensional CA, the life game was representative. The live game was a simulation where many square cells were defined and some of “live cell” was located in the square cells to multiply the lived cells according to some rule, providing non-predictable, complicated and variegated patterns from first simple shape and plain rules. Figure 1 shows the sample of the condition change of the neighborhood cells and the local rule. In the life game, condition change of the live cell at the dispersed time was depended on the conditions of 8 cells surrounded the live cell (Figure 1(a)). The central live cell was disappeared at next step if no live cells were existed around the center cell (Figure 1(b)) and over 3 of the live cell were surrounded the center cell (Figure 1(c)). If 2 of the live cells were existed around the center cell, the condition of the center cell was not changed at next step as shown in Figure 1(d). In the other hand, if 3 of the live cells were surrounded the central non-live cell, the central cell was change to the live (Figure 1(e)). Applying these local rules, the conditions of the cells were changed one after another. Like as the above local rules, the rule to control the concentration change in local portion of soil could be established to obtain more accurate analysis.



(a) Condition of 8 cells surrounded

(b) When no live cells were existed around the center cell, the central live cell was disappeared.

(c) When over 3 of the live cell were existed around the center cell, the central live cell was disappeared.

(d) When 2 of the live cell were existed around the center cell, the condition of central live cell was not changed.

(e) When 3 of the live cell were existed around the center non-live cell, the central cell was change to the live.

Fig.1 Life game

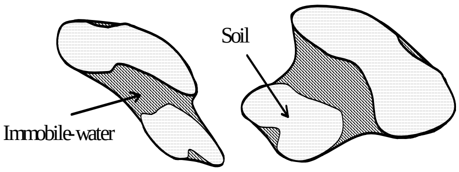


Fig.2 Outline of immobile-water

3. Diffusion and stream of dissolved materials in soil

(1) One-dimensional diffusion equation

Solvent penetrated through soil is flowed gap-space of the soil. The change of the concentration C in the mobile water region where penetrated solution was fluid was express by Equation (1):

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} + \sum_k R_k \tag{1}$$

,where D : diffusion constant, v : flow rate of solvent, R_k : change amount of dissolved materials such as chemical reaction or radioactive decomposition.

However, if solvent was flowed porous media such as soil, the penetrated water was held in the soil-surface pores and in the gap space among the soil particles due to van der Waals foce at the soil surface. Figure 2 illustrates the outline of immobile-water.

The change of the concentration C in the immobile-water region was expressed by Equation (2) if one-dimensional (z-) diffusion was postulated:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} + \sum_k R_k \tag{2}$$

As chloride ions (Cl^-) was hard to adsorb on soil and held stable condition, the concentrations change of Cl^- in the mobile-water region and immobile-water region were expressed by Equation (3) and (4), respectively.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} \tag{3}$$

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{4}$$

To predict the diffusion phenomena of Cl^-, two models in the mobile-water region and immobile-water region should be considered.

(2) Break-through curve from column experiment

To investigate material transport phenomena in soil, the column experiment was carried out where the solution contained the objective material was pored on the top of the soil packed layer in the column and the concentration change of the solute was measure at the bottom of the column. Figure 3 shows an example of representative break through curve, which was obtained from the column experiment. The ordinate of Figure 3 was corresponded to C/C_0 ratio, where C and C_0 were the concentrations of the effluent and the column inlet, respectively, and the abscissa was the penetration time. If the penetration solution obeyed Darcy's law, the stream became identical and piston-flow, as curve of ① in Figure 3. In this case, the penetration solution with the relative concentration of unity was flow out.

If the flow rate of the penetration solution depended on the gap space volume, the diversify-flow was realized as curve ② in Figure 3. In this case, the concentration was gradually changed with time passed and the symmetric breakthrough curve with the center of $C/C_0 = 0.5$ was obtained because the dissolved material was come from the penetration solution with higher rate.

If physical or chemical interaction between the solvent and soil particle was postulated, tailing-flow, ③ in Figure 3, appeared. In this case, the breakthrough curve with tail was obtained because until the relative concentration became unity, more time was consumed due the dissolved material decreased by the physical or chemical interaction. For the column experiment employing chloride ions, the immobile-water was formed and chloride ions were held in the site to delay reaching time to the column outlet, providing the breakthrough curve of ③ in Figure 3.

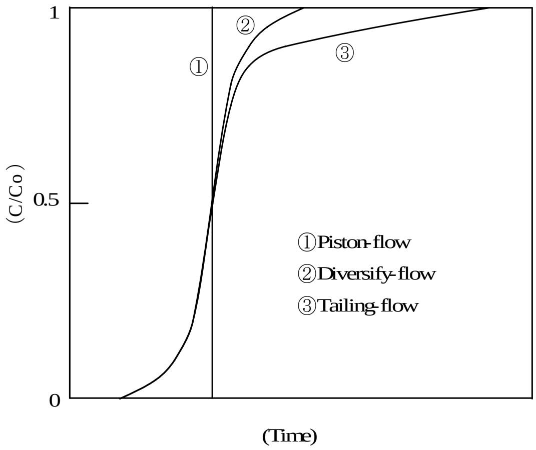


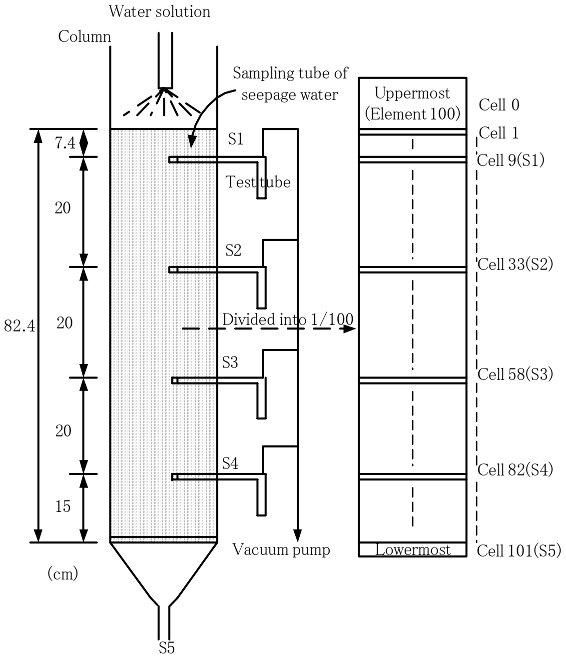
Fig.3 Representative break through curve

4. One-dimensional CA model diffused in soil

In the present study, the column experiment result for chloride ion, which was carried out by the Central Research Institute of Electric Power Industry[7)], was employed as the basic data for simulation. The modeling and the local rule to apply the CA to the soil contamination simulation were described below.

(1) Modeling of soil for applying CA

To simulate the column experiment by the CA, the column height was divided into 1/100 of 0.824 cm from the whole height of 82.4cm as shown in Figure 4(a) and each height region was defined as the cell for the CA. Then, the top and the bottom cells were added to prepare 102 cells totally, where the cells were numbered from the top to the bottom as 0, 1, ･･･, 101 (Figure 4(b)). As the unit height of the cell was 0.824, the measurement position of S1, S2, S3, S4, S5 were corresponded to cell 9, cell 33, cell 58, cell 82, cell 101, respectively.



(a) Column experiment (b) Cell alignment

Fig.4 Cell alignment for the CA

(2) Cell condition

As cell condition, the mobile-water layer and immobile-water layer were postulated. In the mobile-water layer, mobile-water region, where the penetration water was flowed, and soil particle region were existed. In the immobile-water layer, mobile-water region, soil particle region and immobile-water region were existed. The chloride ion solution (Cl:100 μ g/ml) was supplied continuously from the top of the column to transfer in the soil.

To simulate the phenomena by the CA, 100 of chloride ions were postulated to exist in the cell 0. The 100 of chloride ions were transferred from cell 1 to cell 101 applying local rule. The possible chloride ions number existing in each cell, cell 1 – cell 101, was limited to 100.

(3) Local rule for diffusion

a) Material transfer treatment

Diffusion phenomenon was expressed by self-transfer of each chloride ion in the penetration solution. As chloride ions transferred in the penetration solution, the transfer phenomena depended on the condition of the solution. Then, in the modeling of one-dimensional diffusion simulation for the present study, each chloride ion was moved by the probability theory and the probability of chloride movement through one cell was determined according to the condition of penetration solution. The chloride movement probability through one cell was changed according to the mobile- or immobile-water layers to express the change in the diffusion phenomena for both layers.

The simulation was done by the flow chart showed in Figure 5. For each chloride ion, random number was assigned and the chloride ion was postulated to transfer to the next down cell if the random number was small than the transfer probability. All chloride ions were treated once in one step. As the order of the treatment, the treatment was stated from the bottom of cell 101 to the upper cell. The order from the cell 0 to down cells was limited the existing chloride ion number to lead less number of the transfer.

b) Proportion of the immobile-water layer and transfer probability of the element

Not only the proportion of the immobile-water against the whole soil volume but also the ration of the element transfer probability in the mobile- and immobile-water layer (Figure 5, transfer probability1 and 2, respectively) were determined by the following method.

The theoretical mean flow rate of soil-penetrated water in the column experiment was expressed by Equation (5):

$$V = W/(A \cdot \theta) \qquad (5)$$

,where W: water amount, A: cross sectional area of column, θ : water containing ration

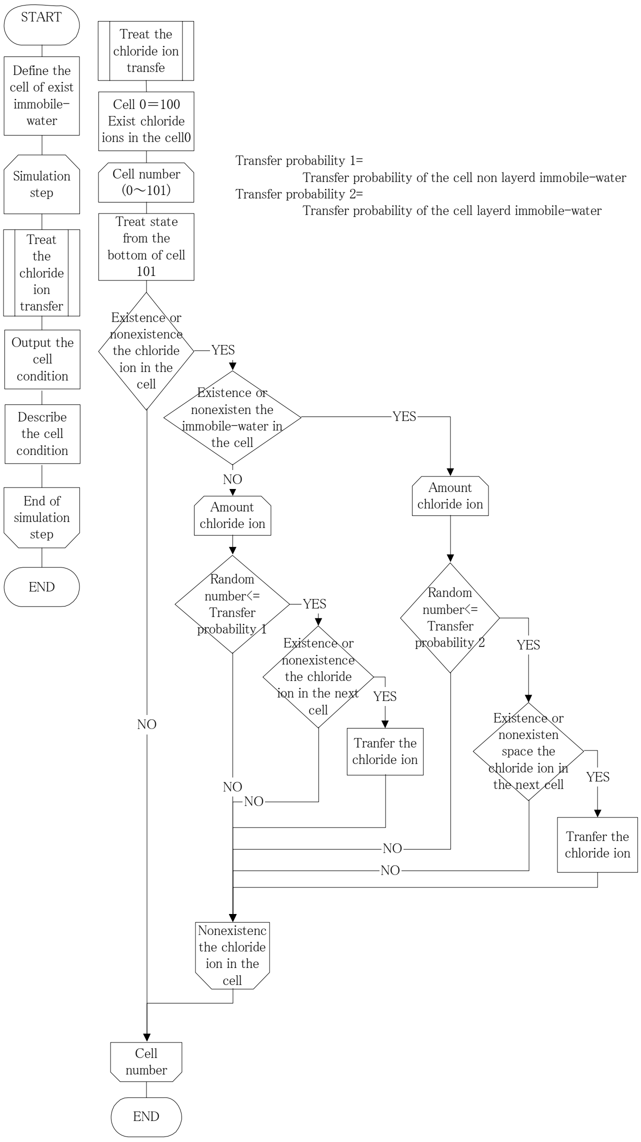


Fig.5 Simulation flow chart

For the column experiment, W=942cm^3/h, A=314cm^2, θ =0.629 were used and the mean flow rate was 4.8cm/h from Equation (5). However, the column height was divided by the time when the C/C_0 in S5 became 0.5 to yield the mean flow rate of 6.5cm/h. The difference in the both mean flow rates was due to that the immobile-water was formed in the column and the effective cross section area decreased to increase the flow rate. The proportion of the immobile-water against the whole water in the soil was postulated to be 26% by means of $(6.5-4.8)/6.5=0.26$, and then the immobile-water layers were assigned in 26 cells out of 100 cells and the mobile-water layers were assigned the residual cells. The element transfer in the mobile-water layer and the immobile-water layer occurred mainly by the mobile water transfer itself and molecular diffusion, respectively, providing the considerably lower transfer rate in the immobile-water layer than that in the mobile-water layer. Postulating that the difference in the element transfer probability in both mobile- and immobile-water layers was due to the proportion of the mobile-water region in both layers, the ratio of the transfer probability was calculated as follows,

Water mobile layer: immobile-water layer = water containing ration : water containing ration (1- proportion of immobile water) = 0.629 : 0.463[7)]

From the mean flow rate of 6.5cm/h and one cell (0.824cm) length of diffusion in one step treatment, the actual time for one step was corresponded to 0.824／6.5＝0.126(h).

For executing the simulation, Java, which was a program language developed by Sun Microsystems Co., was employed. The Java was favorable parallel treatment and easily could be added the treatment items afterward.

5. Simulation results and discussion

Employing the diffusion model in soil and the local rules, the simulation was done 20 times and the mean result of the simulations was compared with the result in the column experiment to verify the applicability of the CA.

(1) Determination of element transfer probability in mobile- and immobile-water layers

As the position of the immobile-water was not known in actual soil, the immobile-water layer was set at random in the CA cells and the element transfer probability was varied into 15, 30, 45, 75, 90 and 99% to execute the simulation. The element transfer probability in the immobile-water layer was adapted to the value described in 4. (3) b).

The time when the $C/C_0=0.5$ in the cell 101 was searched to be closed to that when the $C/C_0=0.5$ at S5 in the column experiment and the transfer probability at that time was obtained. As shown in Figure 6, the transfer probability of 99% and 72.27% in the mobile- and immobile-water layers, respectively, gave the closest result to that in the column experiment. These values for the transfer probabilities were employed in the present study.

(2) Investigation of position for immobile-water layer

Varying the element transfer probability, the simulation was carried out as shown in 5.(1). However, the C/C_0 level of the tailing was lower in all cells and the start time of the curve raising was more delayed at the lower cells. These results were probably due to that the immobile-water layers were set to the upper side and then the transfer rate became to be lower. To concentrate the immobile-water layers in the lower side, the following cells were set to be the immobile-water layers:

Cell number, 50, 59, 60, 62, 65, 67, 69, 73, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100.

As shown in Figure 7, the simulation results were closed to that in the column experiment, showing that the immobile-water layers were existed to concentrate in the lower side in the experiment column.

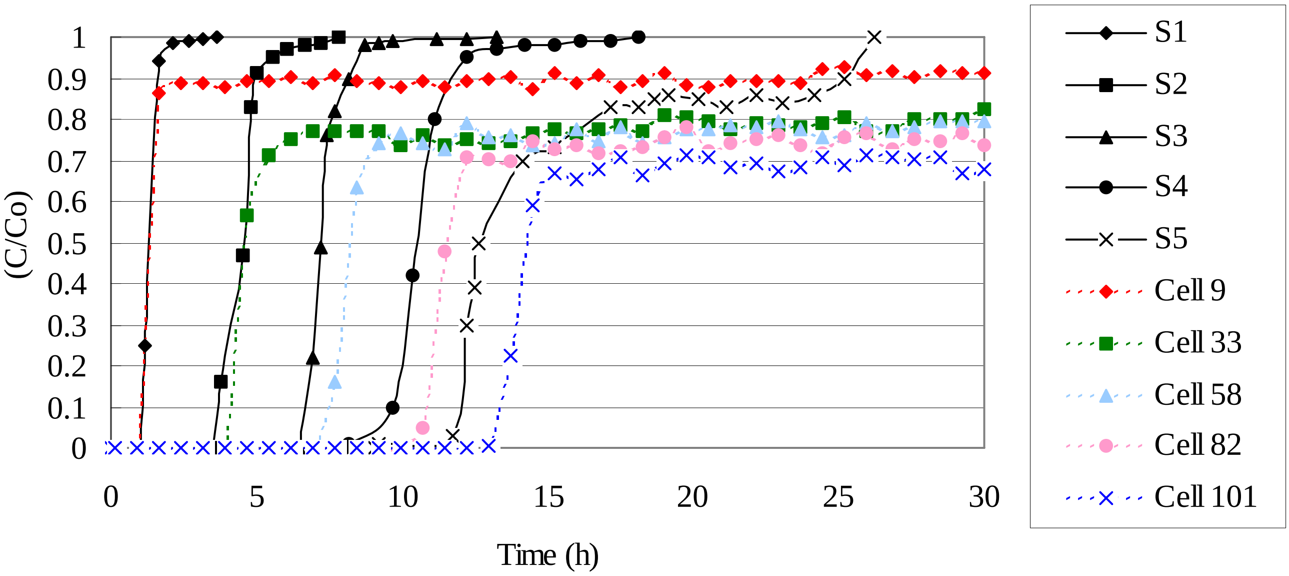


Fig.6 Simulation result of the transfer probability of 99% and 72.27% in the mobile- and immobile-water layers

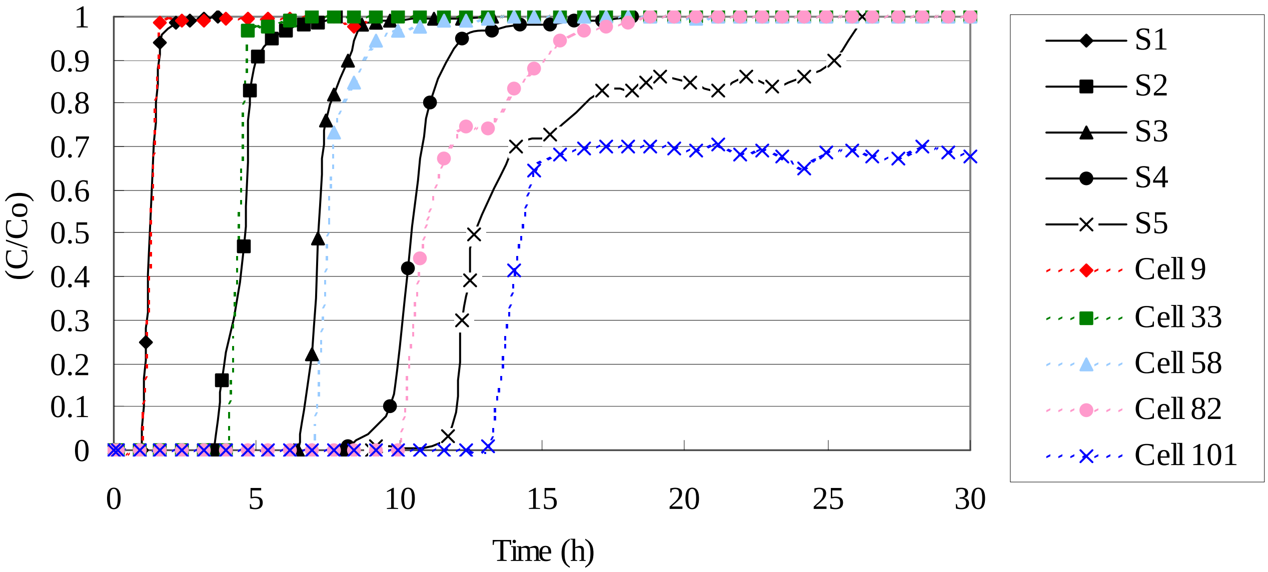


Fig.7 **Simulation result of due to that the immobile-water layers were set to the upper side**

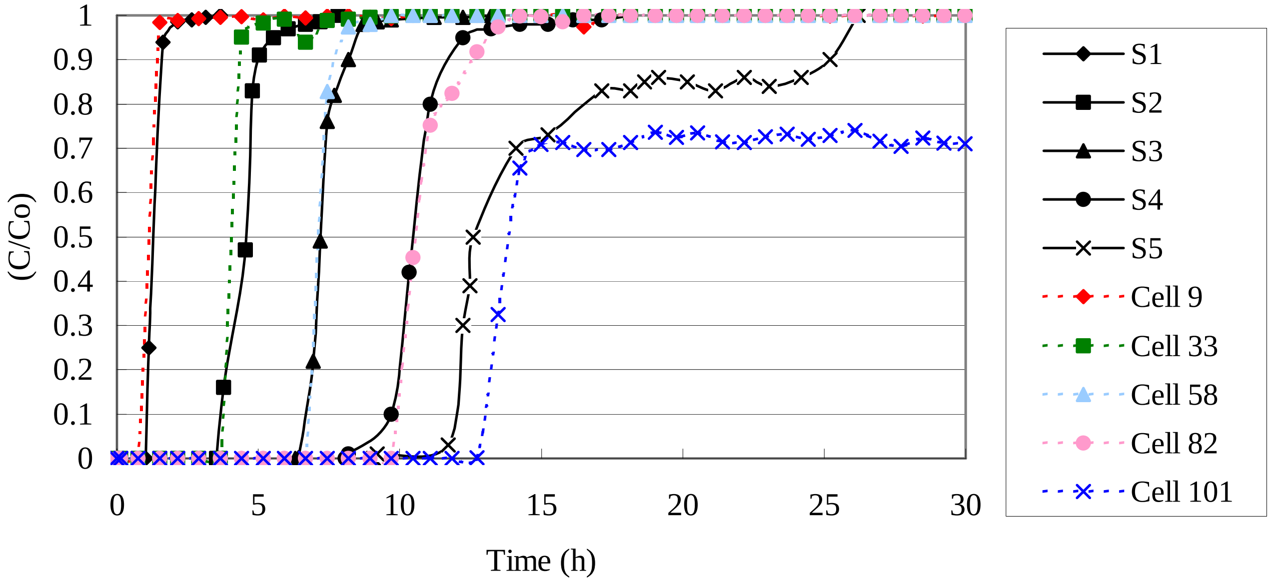


Fig.8 **Simulation result of due to that the proportion of the immobile-water layer were 21%**

(3) Investigation of proportion for immobile-water layer

The C/C$_0$ level in the cell 82 at the start was rather lower though the immobile-water layers were postulated to be in the lower side of the column as described in 5. (2). Postulating that higher transfer probability in the immobile-water layer gave higher C/C$_0$ level of the tailing at the start, higher transfer probabilities were adapted to the simulation but there were no distinct difference in the result where the transfer probability was varied from 72.27 to 75.24%. As another postulation, the C/C$_0$ level of the tailing at the start was expected to increase with decreasing the proportion of the immobile-water layer. Then, decreasing the proportion from 26 to 21%, the simulation result was obtained as shown in Figure 8, where the value at the cell 82 became to be closed to that in the column experiment. The error at the upper cells increased with minimizing the error at the lower cells, showing that better simulation was not expected further. As shown in Figure 4(a), the bottom of the column was shaped as a cone and was not packed with soil. The simulation result at the cell 101 was sufficiently expressed the experimental result at the S5 though no volume data for the bottom corn.

6. Conclusion

In this paper employing the CA, the authors proposed the diffusion model for chloride ion postulating the mobile- and immobile-water layers to estimate the transfer phenomena of contaminated materials in soil. The simulation using the model was verified to reproduce characteristic phenomena of the tailing in the breakthrough curve, which was obtained in the column experiment. Moreover, it could be shown to estimate the distribution of the immobile water in the column, which was difficult to obtain only by the experiment. The CA was possibly applied to the simulation of soil contamination.

Chloride ion, which was hardly accepted an interference from soil penetrated water, was employed in the present paper, providing the basic diffusion expression. By considering the local rules such as adsorption/desorption with soil particles and vaporization/dissolution, more realistic simulations dealing with heavy metals and/or volatile organic matters should be enabled.

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