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A method about setting CTRW model parameters for the prediction of the behavior of adsorptive substance

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Recently the problem of ground water pollution attracts more attention. The continuous time random walk (CTRW) model, which is one of the methods to evaluate contamination, has been noticed because it can describe the complex behavior of substances in heterogeneous porous media. However, implicating the CTRW model to real problems, values of the model parameters cannot be fixed *a priori*.

Now when we use the CTRW model, we determined the values of model parameters by trial and error. This method takes labors due to the lack of criteria for deciding parameters. Meanwhile, the Advection Dispersion Equation (ADE model) is conventional method for describing the behavior of substances in groundwater. However, it is reported that the ADE model cannot describe the behavior of substances in heterogeneous porous media. On the other hand, the ADE model is relatively easy to be used because it consists of measurable parameters. Therefore, in the present study, we concentrate on studying the relationship between the ADE model parameters and the CTRW model parameters and finding the method of determining the CTRW parameters from measurable experimental parameters.

In the ADE model, the model parameters are threefold; the velocity v (m/s), the dispersion coefficient D (m^2/s) and the retardation factor R. These values can be solved from experimental values. On the other hand, in the CTRW model needs following three parameters; coefficient a, the fine distance dx(m) and the fine time dt (s). In the CTRW model, we regard the migration of the substances as the jump of particles and describe the heterogeneity of porous media by giving distribution of waiting time t between each jumps. The waiting time describes how long staying at a site before a particle jumps. In this study, we use the probability density function P(t) proportional to t^{-a}.

The value of a has a deep relationship with the behavior of relevant system. The dx describes how far the particle moves in each jump and the dt describes how long it takes in each jump.We concentrated on the parameters mentioned above and conducted the numerical experiment between the ADE model and the CTRW model. As a result, we found that the relationship of two can be described in following equations.

$dx = D/(v*k*<t>)$

$dt = D/(v^2*k*<t>)$

The term k is a coefficient approximated by each a and can be found experimentally. The term <t> describes the mean of waiting time and can be solved in each a.

In addition, we conducted a series of column test to obtain diffusion behavior in a laboratory scale. Toyoura sand was filled in the equipment as porous media, and Zn and Pb was used adsorptive tracer. We observed how the concentration of tracer changed from the difference of adsorption strength and compared the data between Zn and Pb using by the equation mentioned above. In consequence, we found that the most suitable a to experiment data can be estimated from the retardation factor R.

Keywords: soil pollution, anomalous transport, continuous time random walk, adsorption, heterogeneity, heavy metal