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Multi-Scale Modeling for Anomalous Diffusion in Inhomogeneous Media -Creating an Interdisciplinary Platform for Taking Aim at Mathematical Innovation-

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Abstract

Nippon Steel & Sumitomo Metal Corporation recognizes that mathematics is a powerful language that can capture the essence of a variety of problems. This is why the collaboration is in the process of creating an interdisciplinary platform to encourage mathematical innovation. This platform is to serve as a framework for the coming together of mathematicians and engineers to contemplate social problems and to take voluntary actions.

The scientific topic revolves around anomalous diffusion in soil. This is a typical multi-scale modeling subject since the field scale is macro, i.e., 100 m-10 km while the pore size of the soil is micro, i.e., about 100 μm. Multi-scale modeling is in great demand in social and industrial problems, but the mathematical theory has not yet been fully developed.

It is often the case with mass diffusion in a porous medium such as soil that the numerical simulations using traditional advection diffusion equations fail to predict the observation results of a real phenomenon observed in the field or in laboratory tests. The numerical experiments using the continuous time random walk (CTRW) approach, predict that the mean squared displacement of particles grows in proportion to the fractional power of time.

The first scenario deals with multi-scale modeling from a macro-scale viewpoint. The CTRW approach is linked with the fractional differential equation (FDE) in terms of time. This means that anomalous diffusion depends on the degree of history to be retained from the initial time to the current time. The smaller α is, the more history will be retained. We can combine the physical meaning of alpha (which is due to possible obstacles that delay the particle's jump) with mathematical reasoning.

The second scenario takes a micro-scale viewpoint. Thus, how do we combine the microstructure with the mechanism for determining the value? What are the geometric invariants? How do we combine the geometric invariants with the PDE in a mathematical framework? These are our next concern. We consider the relationship among the CTRW approach, the FDE, and the alpha value through the characterization of the geometric features of the specimens of a 3D CT-image.

The third scenario takes a multi-scale viewpoint. Here, a deductive reasoning is considered to derive a FED using the homogenization method..

Introduction

The steel making process requires control of a diverse range of phenomena involving mathematical applications for problem solving and modeling.

"Mathematics for industry" is aimed at extracting universal fundamental principles behind various natural phenomena and engineering problems, and crystallizing them into mathematical structures, and is essential for applying mathematics for industrial technology.

A methodology based on the mathematical thinking enables us to construct mathematical models that describe the essence of a phenomenon selectively. Such mathematical models serve as important basis for understanding and controlling a phenomenon. When a mathematical model describes the essence of a phenomenon as simply and comprehensibly as possible (a minimum necessary model), it becomes easier for engineers and researchers from a variety of technical fields to study, and it becomes easier to conceive ideas that can lead to innovations.

Nippon Steel & Sumitomo Metal Corporation has globally collaborated with mathematicians for decades and resolved industrial problems by enhancing practical insights with mathematical reasoning. Engineers in Nippon Steel have learnt how to understand the phenomena in the steel-making process only by the rules of pure logic, not by a posteriori ad hoc ways. On the other hand, mathematicians in universities have learnt how to link mathematics with the physical reality of the phenomena.

As a result, the collaborative research is playing a major role in mathematical innovation to broaden the diverse range of applications in mathematics and cultivation in both industry and the field of mathematics.

Collaboration Style

Figure 1 shows our style of collaboration with engineers and mathematicians in the case of Nippon Steel & Sumitomo Metal Corporation and the University of

Tokyo. We formed international task force teams made up of faculty members, post-doctoral fellows and doctor course students. Team members are selected flexibly to create a task force according to the characteristics of the task. Our collaboration is composed of six indispensable phases.

The first is “intuition and expertise” from industry. Intuition and expertise can be carried out exclusively by insight based on observation of phenomena in the manufacturing process. The insight should be enhanced by mathematical reasoning. The second is “communication.” Communication is bilateral translations: the translation of phenomena to mathematics and the translation of mathematics to phenomena. Engineers in industry need to understand real problems on site, express them in the language of physics, and offer possible model equations to mathematicians. Mathematicians explore the underlying mathematics to the model equations. This forum for communication through the interpretation of phenomena is extremely important in order that engineers and mathematicians may reach a common understanding of the nature of the problem and the mathematical components. The third is “logical path.” This corresponds to the extraction of mathematical principles from phenomena. Better communication can create a more logical path. The fourth is “analysis of data.” This means reasonable and quantitative interpretation of observations carried out on site. This enables us to extract the essence of phenomena. The fifth is “manufacturing theory.” This means the integration of logical paths from viewpoints of operation and economic rationality on site. The last is “activation to mathematics.” Motivation for mathematicians has launched new mathematical research fields.

We, engineers in industry, have been eager to free ourselves from restrictions in our conventional thinking by making full use of mathematical reasoning that is free from specific industrial fields, through wider borderless collaborations. We have examined various conjectures by mathematicians and gained better practical solutions and further utilized analysis results. By repeating such phases of collaboration many times, we are able to pursue economic rationality, and mathematicians are able to find new results and describe them as theorem for future wider uses. It is important that mathematicians work not only for mathematical interests but also for the economic rationality through teamwork with engineers from a long-term point of view.

The cultivating interface between mathematics and industry has come into being as a forum for communication with the mathematicians mentioned above. Communication between the team members who are engineers in industry, and faculty members, post-doctoral fellows and doctor course students in university mathematical departments, has enhanced their communication skills day by day. As a result, several new themes have been launched.

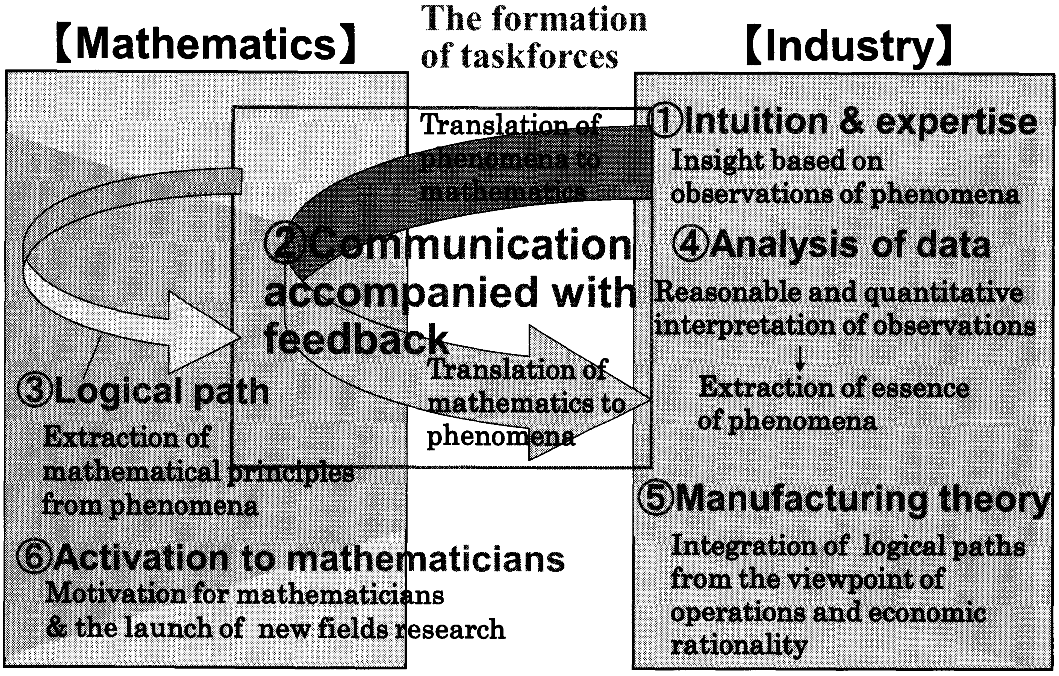


Fig.1 Collaboration with engineers and mathematicians in the case of Nippon Steel and the University of Tokyo

Example of interdisciplinary collaboration

Figure 2 shows a challenge faced by Dr. Yuko Hatano. She is an associate professor affiliated with the University of Tsukuba whose major is Risk Engineering, and she had already collaborated with Nippon Steel on another subject.

The objective is to predict the progress of soil contamination. It is often the case with mass diffusion in a porous medium such as soil that numerical simulations using traditional advection diffusion equations fail to predict observation results of a real phenomenon observed in the field or laboratory tests. For instance, there are cases where actually the concentration is beyond the environmental standard as shown in Fig.3, even when a simulation indicates that the concentration of the pollutant is below the relevant environmental standard and the danger of soil pollution is unlikely. Diffusion not following the prediction based on such a simulation is called anomalous diffusion, in contrast to the traditional diffusion equations, and is often observed in different manners with various substances in the soil or atmosphere in the real environment.

The above is the kind of problem that we encounter when numerically simulating a soil system in which voids are distributed unevenly between particles, using a grid for calculation larger than the voids. This type of problem will not occur when the grid spacing is smaller than the voids between soil particles, for instance, about 0.1 mm. However, since several kilometers or more is the normal scale for environmental studies, in view of computer load the use of such a fine grid for a three-dimensional case is extremely difficult, and is practically unsuitable for on-line field analysis. Moreover, whereas a model test covers a time scale of as short as minutes to days, the prediction of a real environmental problem must deal with a time scale as large as a few years to tens of years.

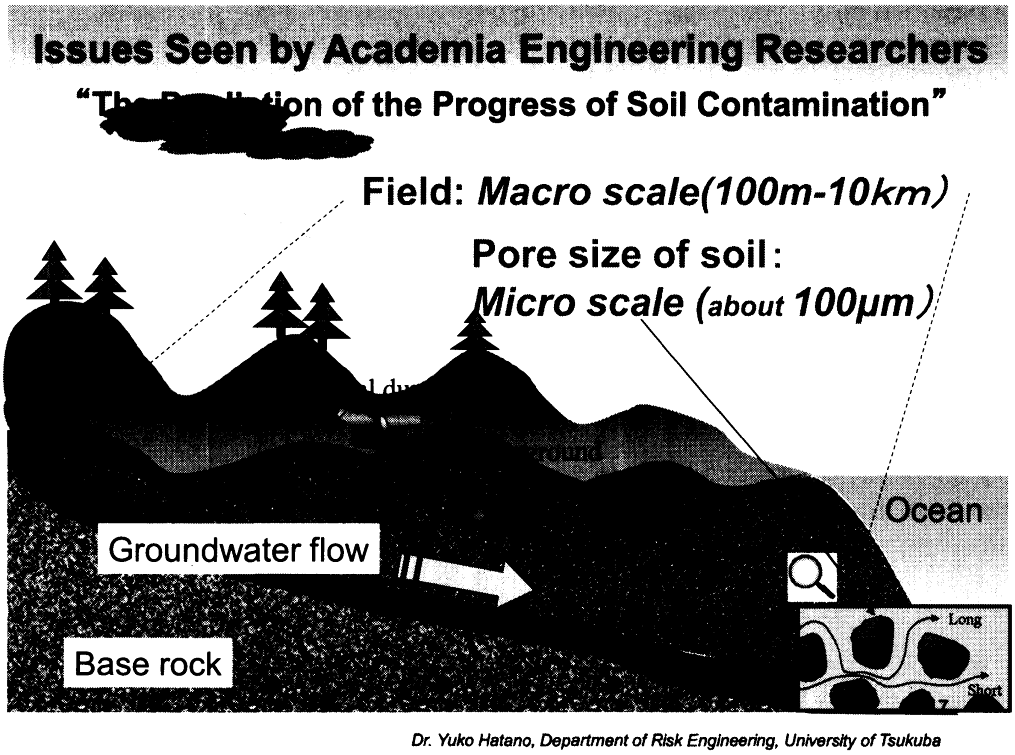


Fig.2 Prediction of soil contamination on a large scale and over a long term

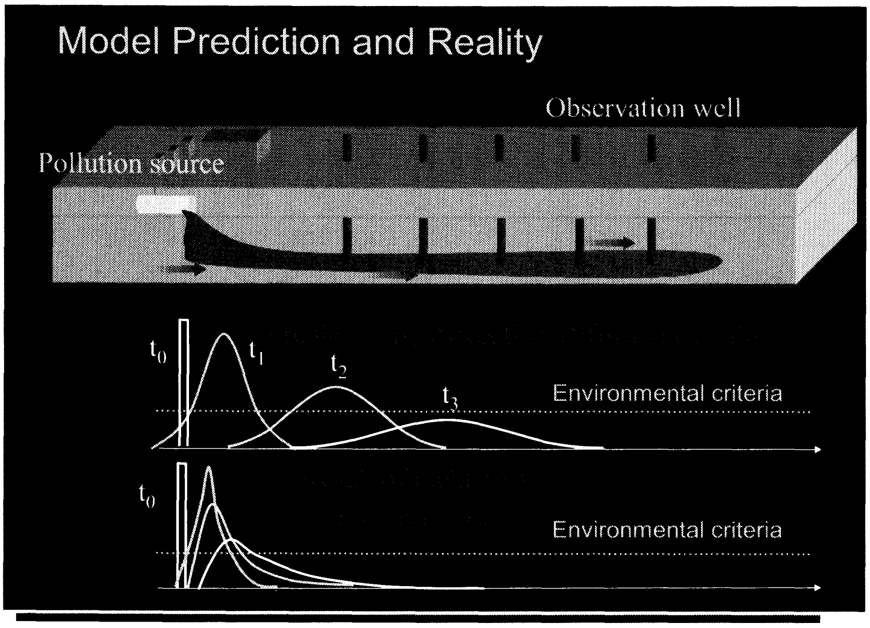


Fig.3 Comparison between model prediction and results of field tests

Although we have to treat widely varied sizes of data obtained through physical and numerical tests based upon different scales of space and time, the scaling law allows us to combine those data together in accordance with principles of phenomena.

Large-scale numerical simulation is the principal method for the dynamic analysis of substances in any environmental medium: air, water or soil. Many detailed chemical and biochemical reactions are incorporated in the program codes for environmental simulation, and as a result, simulation programs seem to be becoming increasingly complicated these days. While a great number of numerical simulations are conducted on environmental issues, it is often difficult to tell whether each of such simulation results is valid, which fact is most serious for the problems.

Therefore the present study aims at dynamic prediction of environmental phenomena not totally depending on conventional numerical simulations but also employing mathematical methods typically such as scaling law. Toward this end, it is desirable to create a new field of environmental study involving mathematicians.

Launch of new research field in mathematics

A stochastic method employing random walk in consideration of the distribution of the waiting time of particles is used for describing mass transfer in soil. The stochastic method is called as CTRW that stands for Continuous Random Walk). The CTRW method has been effective when applied to the small space dealt with in laboratory tests, but the limitation on the number of particles is a bottleneck due to the limit of computer capacity, and thus the method cannot respond effectively to more pragmatic requirements of calculation in a larger volume of space.

On the other hand, some fields of physics and engineering employ numerical simulation based on a diffusion equation that includes a fractional-order derivative in time. While the concept of a fractional-order derivative can be traced back to as long ago as Leibniz (see [2]), a theory of partial differential equation that is applicable to such numerical simulation has not yet been established, and the application of such a method has so far been limited to very special cases where the space has only one dimension. It is reported in the literature [3] that, according to the scaling law to the effect that the root mean square of the displacement of particles is in proportion to time raised to the *k*th power (t^k), the stochastic method using the random walk mentioned earlier is closely related to the Fokker-Planck equation, which leads to a fractional-order derivative:

$$(\partial/\partial t)^k u(x, t) = \nabla \cdot (\kappa \nabla u(x, t)) - \mu \cdot \nabla u(x, t),$$

where $u(x, t)$, κ and μ are the probability density function of particles, their diffusion coefficient, and mobility acting on them, respectively. It is expected that a scaling law combines stochastic methods such as the random-walk model for anomalous diffusion with the theory of partial differential equation including a fractional-order derivative to form a new field of research for mathematical concept and methodology. In [1], we discuss a related topic with such a theory.

Besides the above, Hatano et al. found that a formula empirically derived from two short-term atmospheric pollution cases (emission of inert gas Kr-85 from a nuclear plant in U.S.A. and the data of aerosol collected by an international team on global warming in the Arctic Ocean region) can describe the behavior of the pollutant of a long-term atmospheric pollution case (the accident of the Chernobyl Nuclear Power Plant) reasonably well [4], [5]. The formula is also written as a scaling law, but it is not yet been fully clarified why the formula has such a form.

Figure 4 shows that CTRW is linked to the fractional order PDE in terms of time [6]. This means that anomalous diffusion depends on the degree of history to be retained from the initial time to the current time. For smaller α, more history will be retained. We can combine the physical meaning of alpha (which is due to stems from possible obstacles that delay the particle's jump) with the mathematical reasoning. This is a typical example of a problem-solving type that is mathematically based. We present an analytical description that mathematically explains the facts discovered by the experiments.

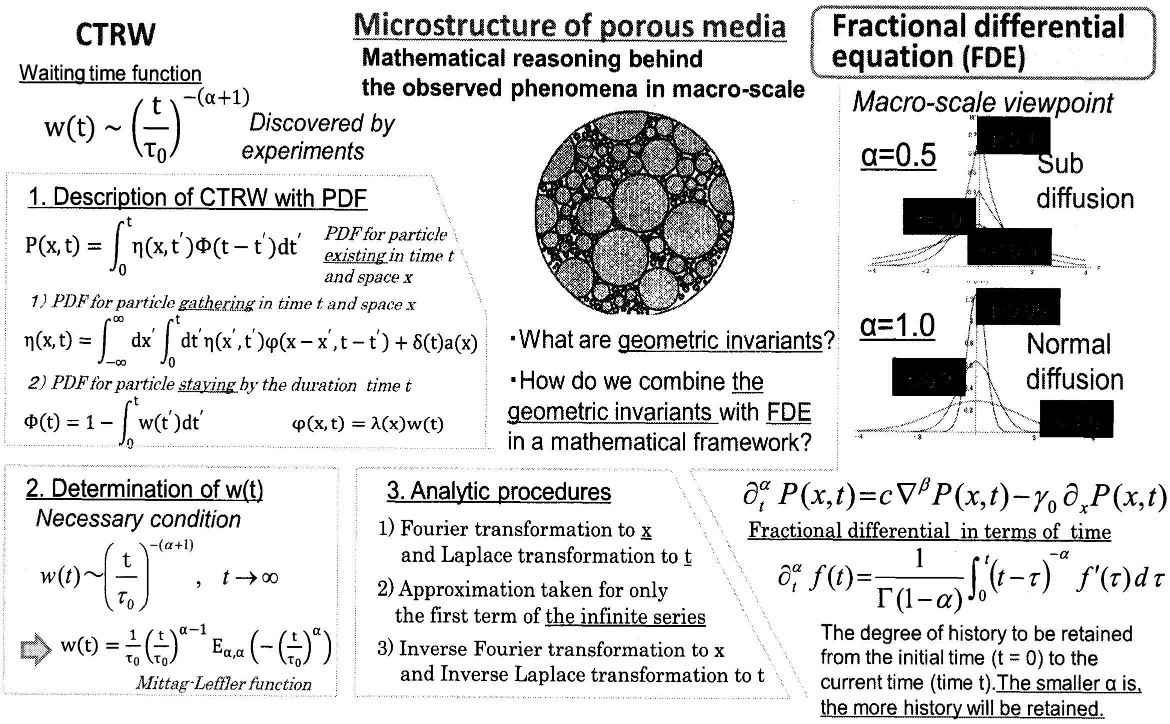


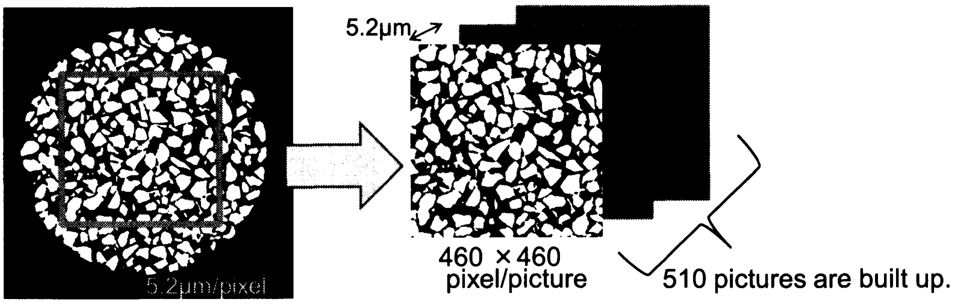
Fig. 4 Analytical descriptions used to mathematically explain the facts discovered by experiments

The approach of the above-mentioned case is based on a macro-scale viewpoint, and is the first scenario for obtaining a multi-scale model. Thus, our next steps involve determining: (1) how to combine the microstructure with the mechanism for determining the alpha value. (2) the geometric invariants, and a method for combining the geometric invariants with the PDE in a mathematical framework. A micro-scale viewpoint will be used.

Figure 5 shows the second scenario used to obtain a multi-scale model. We can use the geometric information of the real sand specimens taken by a 3D CT-image. There are two kinds of dimensions that are used to consider the geometric invariants, namely the geometric dimension, which corresponds to the fractal dimension d_f, and the analytical dimension, which corresponds to the spectral dimension d_s.

Our concern is determining how to combine these geometric invariants with the fractional order PDE in a mathematical framework. Figure 6 shows an approach to obtaining the relationship among the fractal dimension d_f, the spectral dimension d_s and the fractional differential order α. Equation (7) in Fig shows the conclusion.

Characterization of the geometric features of the specimens of 3D CT-image (a micro-scale viewpoint)



1) Geometric dimension ⇒ Fractal dimension d_f

2) Analytic dimension ⇒ Spectral dimension d_s

Fig. 5 The second scenario for getting at a multi-scale modeling [7]

The behavior of the mean volume V occupies by a diffusion particles initially concentrated on a given site x is given by the mean squared displacement and the fractal dimension.

$$V(x,r) \sim r^{d_f} \sim \left(\sqrt{\langle x(t)^2 \rangle}\right)^{d_f} \quad (1) \qquad V(x,r) := \mu(B(x,r)) \quad B(x,r) := \{y \in V \mid d(x,y) < r\}$$

V(x, r) is the Riemannian volume of a geodesic ball B(x,r).

M. Barlow and E. Perkins, Brownian motion on the Sierpinski gasket, Probab. Th. Rel. Fields, 79 (1988), showed that the following heat kernel takes place for a large variety of fractal sets;

$$p(x,y,t) \sim t^{-\frac{d_s}{2}} \exp\left(-\left(\frac{d(x,y)^{d_w}}{ct} \right)^{\frac{1}{d_w - 1}} \right) \quad (2)$$

In the case of y=x,

$$p(x,x,t) \sim t^{-\frac{d_s}{2}} \quad (3)$$

We assume that

$$p(x,x,t) \sim V(x,r)^{-1} \quad (4)$$

With Eq. (1), Eq. (4) and Eq. (3), we obtain that

$$\langle x(t)^2 \rangle \sim V(x,r)^{\frac{2}{d_f}} \sim p(x,x,t)^{-\frac{2}{d_f}} \sim \left(t^{-\frac{d_s}{2}} \right)^{-\frac{2}{d_f}} \sim t^{\frac{d_s}{d_f}} \quad (5)$$

Numerical experiments using CTRW say that

$$\langle x(t)^2 \rangle \sim t^{\alpha} \quad (6)$$

By comparing Eq. (5) and Eq. (6), we have

$$\alpha = \frac{d_s}{d_f} \quad (7)$$

Fig.6 Relationship between d_f, d_s and the fractional differential order α conjectured by Physicists [8]

Figure 7 compares the diffusion behavior between of small-scale experiment and that of large-scale one. The result of the small-scale experiment shows that the diffusion follows an advection-diffusion equation (ADE) that corresponds to the normal diffusion. The result of the large-scale experiment differs from results obtained using the ADE, and it also cannot be completely explained using the CTRW method. We need a scaling law to combine laboratory experiments with field scale.

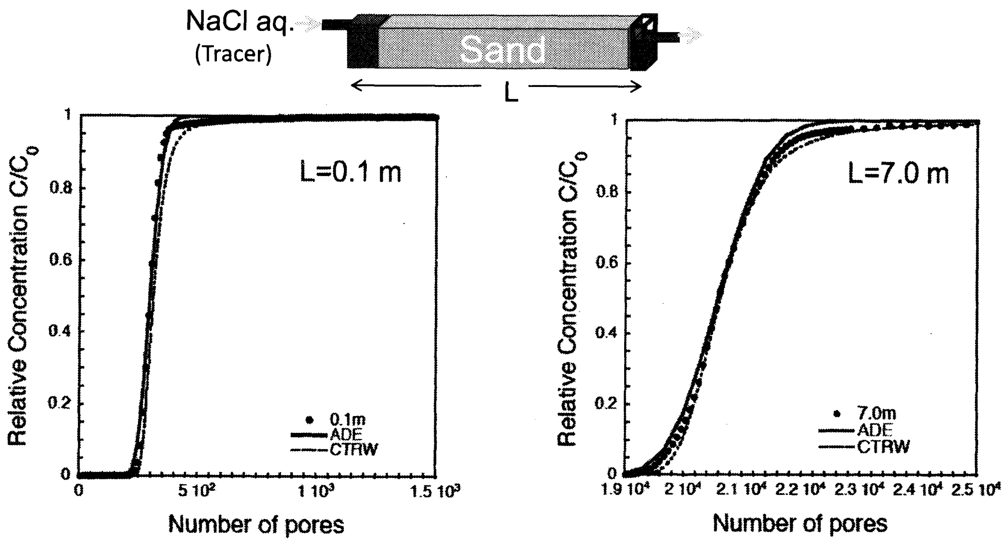


Fig. 7 Comparison of diffusion behavior between small scale experiment and large scale one provided by Dr. Yuko Hatano affiliated with the department of risk engineering, University of Tsukuba

Figure 8 shows the third scenario used to obtain a multi-scale model. This is a deductive approach that uses the nature of mathematics. We use the homogenization method proposed by J.L. Auriault and J. Lewandowska[9].

In Figure 8, Ω is composed of periodic components of a microcell. The governing equation in Ω are given by Eqs. (1) to (3).This PDE is a normal diffusion type. D_m represents the diffusion coefficient of Media M which corresponds to solid particles. On the other hand, D_f is the diffusion coefficient of Media F, which corresponds to air space. Eq. (5) shows the relationship between D_m and D_f. The ε is a homogenization parameter. When ε becomes zero, the relationship in Eq. (5) Plays an important role in the appearance of the memory term in the homogenization Eq. (6). This memory term appears to correspond to the fractional differential in terms of time in FDE in Figure 4.

Deductive reasoning to derive the fractional differential equation using the homogenization method (a meso-scale viewpoint)

$$\begin{cases} \partial_t c^\varepsilon - \nabla \cdot \left(D(x/\varepsilon)\nabla c^\varepsilon\right) = 0 & in\ \Omega \times (0,T) \quad (1) \\ c^\varepsilon(x,0) = c_0(x) & in\ \Omega \quad (2) \\ \partial_\nu c^\varepsilon = 0 & on\ \partial\Omega \times (0,T) \quad (3) \end{cases}$$

Ω is composed of periodic components of a microcell.

where

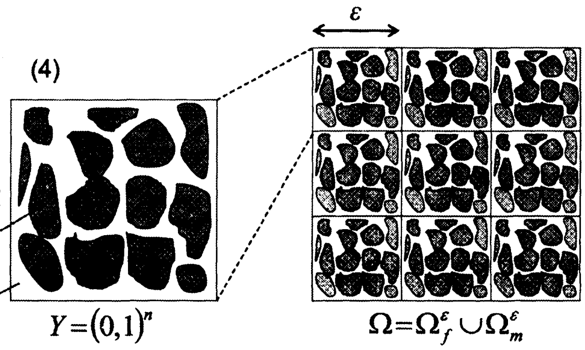
$$D(y) = D_f(y)1_F(y) + D_m(y)1_M(y) \quad (4)$$

$$D_m / D_f \cong \varepsilon^2 \quad (5)$$

The ratio of the two effective diffusion coefficients is defined in terms of the power of the homogenization parameter ε.

Media M (soil particles): D_m

Media F (air space): D_f



When ε goes to zero, c^ε converges to the solution of the following homogenized equations.

Memory term

$$\begin{cases} \partial_t c + \int_0^T K(t-\tau)\partial_\tau^2 c\, d\tau = \nabla \cdot \left(D^{eff}\nabla c\right) & in\ \Omega \times (0,T) \quad (6) \\ c(x,0) = c_0(x) & in\ \Omega \quad (7) \\ \partial_\nu c = 0 & on\ \partial\Omega \times (0,T) \quad (8) \end{cases}$$

Where D^{eff} is determined by D_m, D_f, and the shape of M;

The memory function $K(t)$ is an inverse Laplace transform of the function (9), where $k(y,p)$ is a solution of Eq. (10) and (11)

$$(\mathcal{L}K)(p) = \frac{1}{p}\int_M k(y,p)dy \quad (9)$$

$$\begin{cases} \nabla_y \cdot \left(D_m \nabla_y k(\cdot,p)\right) = p\left(k(\cdot,p) - 1\right) & in\ M \quad (10) \\ k(\cdot,p) = 0 & in\ \partial M. \quad (11) \end{cases}$$

What shape of M leads to a similar effect like the fractional differential?

Our conjecture

$$\partial_t c + f(\partial M)\partial_t^{1/2} c = \nabla \cdot \left(D^{eff}\nabla c\right)$$

Perimeter ∂M probably plays an important role.

Fig.8 The 3rd scenario for getting at a multi-scale modeling provided by Dr. Masaaki Uesaka who is affiliated with Graduate School of Mathematical Science, The University of Tokyo

Thus, through the collaboration of mathematicians and engineers from both academic and industrial fields, our study establishes the fundamental logical structure that lies behind the scaling law observed in the behavior of pollutants in different environmental media such as soil and atmosphere, and thus clarifies the universal characteristics of the scaling law.

Future Plan

In industrial practice, a reduced-scale model is constructed to analyze a phenomenon that takes place in real-size equipment, significant physical values for the phenomenon in question are described by dimensionless numbers, and the dimensionless numbers obtained from the model analysis are made to match with those of real-size equipment. This matching operation secures the similarity of the dynamic physical values between the model and real-size equipment. This similarity refers also to the scaling law. It has been found from the above viewpoint of scaling law that, in addition to the physical values such as time and length which have been conventionally used for scaling up, the fractional powers in the differentiation of time and space are essential. This means that mathematics is expected to present a new "angle of view" for the scaling law that deals with inhomogeneous media. Practically, environmental analysis deals with a scale of several kilometers or more in size. In this relation, establishment of scaling laws including an a priori choice of an exponent will make it possible to appropriately use results obtained through reduced-scale tests and clarify a real phenomenon across a large space.

By establishing scaling laws and developing mathematical methods based thereon, we can significantly reduce costs for producing high-quality products as well as energy consumption and CO_2 emission by improving production efficiency in various problems of manufacturing industries such as monitoring of sintering processes, reactions in a blast furnace, and other metallurgical reactions in steel-making processes.

Scaling laws and mathematical methods are applicable also to a wide variety of fields such as chemical engineering, mechanical engineering, geotechnical engineering, biotechnology, etc., and therefore, the establishment of such scaling laws is expected to be useful in remarkably accelerating the development of science and technology through the solution of important industrial problems.

Furthermore, the concept of scaling law combining micro- and macroscopic aspects is closely related to that of multi-scale modeling, the application of which is rapidly expanding in material science, chemistry, and other widely varied fields. The present study is expected to lead to proposals of new mathematical concepts and methodologies for multi-scale modeling, bringing about new problem recognition and methodology to mathematics.

"Mathematics for industry" will be the key for combining mathematics with industrial technology. Mathematical science can be understood as mathematics for nature; it is aimed at extracting fundamental principles behind different natural phenomena and engineering problems, and crystallizing them into mathematical structures.

Beyond the simple numerical operation of physical model equations, a methodology based on the principles and rules of mathematics makes it possible to construct mathematical models that describe the essence of a phenomenon selectively. Such mathematical models serve as important basis for understanding and controlling a phenomenon. When a mathematical model describes the essence of a phenomenon as simply and comprehensibly as possible (a minimum necessary model), it becomes easier for engineers and researchers from a variety of technical fields to study, and it becomes easier to conceive ideas that can lead to innovations.

In order to construct such a minimum necessary mathematical model that describes the essence of a phenomenon efficiently, a framework is required for the joint work of mathematicians and engineers from academic and industrial fields where they can thoroughly discuss subject phenomena and define suitable targets and milestones for different study stages. In addition, it is indispensable to mutually confirm work progress. At present, however, applied mathematics in Japan, compared with other developed countries, seems to lack such teamwork experience that helps to combine a phenomenon with mathematical methodology. In order to solve a problem as promptly as required in industry, it is too late to begin studying methodology after posing of the problem. It is necessary to continue to improve the skill to combine a phenomenon with mathematical methodology for its prompt application, and in this respect, each individual must improve their qualification to be "the right person" who can meet the above conditions and the role.

It is desirable that both mathematics and industry foster people capable of working jointly with each other from the viewpoint of "mathematics for nature" through academic-industrial collaboration. Towards this end, it is necessary to create a new framework independent of the structure of present industry and academic organizations. We must reinterpret and reconstruct the fundamental concept of manufacturing based on field practice, which constitutes the competitive edge in developed countries, from the standpoint of mathematical methodology while learning about interdisciplinary collaboration from abroad. By so doing, we will be able to command the most advanced industrial technology of the world.

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