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NUMERICAL SIMULATIONS OF WATER ADSORPTION MODEL BY FINITE ELEMENT METHOD WITH ADAPTIVE MOVING MESH METHOD

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Abstract. A mathematical model of water adsorption phenomena is formulated by Aiki, Murase, Sato and Shirakawa in [4], and mathematical results are shown in [5], [6], and [7]. On the other hand, numerical simulations have been only given in [4] by experimental approximating technique without any sufficient mathematical proof. The numerical simulations gave the graph of the solution for water adsorption model drawing hysteresis-like loops under certain conditions. It is a suitable behavior with phenomenon point of view. In this paper, we configure a numerical scheme given by the finite element method with the adaptive moving mesh method, and we confirm the validity of the numerical results in [4].

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1 Introduction

Water adsorption is one of the phenomena observed in the concrete carbonation process. As already well known, concrete is a porous medium, and it adsorbs moisture liquid and moisture vapor in the air into holes in concrete. The adsorbed vapor makes concrete neutral, and neutralized concrete becomes not be able to protect reinforcing steels and buildings from corrosion. Thus, it is known that concrete carbonation is a big issue in civil engineering field.

The adsorption phenomena is studied by many civil engineers. For example, Maekawa, Ishida, Kishi [1], and Maekawa, Chaube, Kishi [2] showed properties appearing the adsorption phenomena. The following Figure 1 is a graph of relationship between saturation and humidity which is given by real experiment.

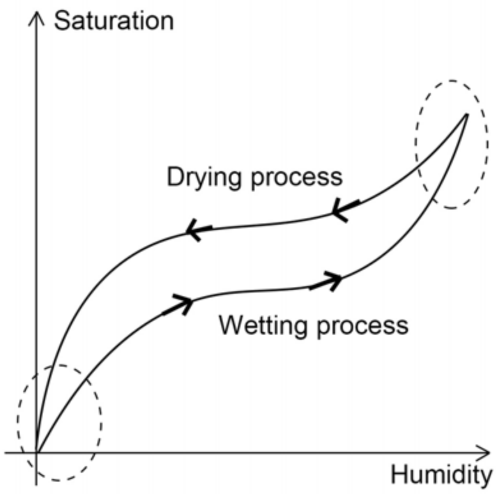

Figure 1: behavior of adsorption phenomena

When the humidity of vapor in the air is high, the concrete takes in vapor, and saturation of water in the concrete becomes higher. In this wetting process, the relationship of saturation and humidity follows the lower curve in Figure 1. In this drying process, the relationship of the saturation and the humidity return back to the left side, and follows the upper curve in Figure 1. As seen in the graph, the relationship follows different paths in the wetting process and the drying process. Hence, the relationship draws the counterclockwise hysteresis-like loop as in Figure 1.

Aiki, Murase, Sato and Shirakawa proposed the following mathematical model of adsorption phenomena (S) in [4] to analyze the phenomena, mathematically. (S) is an evolution system of partial differential equations as a free boundary problem in the one dimensional space.

$$\rho_v u_t - \kappa u_{xx} = 0 \quad \text{on } \ Q_s(T), \tag{1}$$
$$s'(t) = \alpha(s(t), u(t, s(t))) \quad \text{for } \ 0 < t < T, \tag{2}$$
$$u(t, L) = g(t) \quad \text{for } \ 0 < t < T, \tag{3}$$
$$\kappa u_x(t, s(t)) = (\rho_w - \rho_v u(t, s(t)))s'(t) \quad \text{for } \ 0 < t < T, \tag{4}$$
$$u(0, x) = u_0(x) \quad \text{for } \ s_{(0)} < x < L, \tag{5}$$
$$s(0) = s_{(0)}, \tag{6}$$

where $0 < T < \infty$, κ, ρ_v, ρ_w are positive constants, $Q_s(T) = \{(t, x) \mid s(t) < x < L, 0 < t < T\}$, g is a given function on $(0, T)$, α is a given function on $\mathbb{R}^2$, u_0 is a initial function on $(s_{(0)}, L)$, and $s_{(0)}$ is a initial value of the free boundary.

We call a pair of unknown functions $\{s, u\}$ a solution of (S) satisfying (1) to (6) and some regularity conditions. For this system, there exist some mathematical results. Sato, Aiki, Murase and Shirakawa [5] proved existence and uniqueness of local solutions in time, Aiki and Murase [6] proved existence and uniqueness of global solutions in time and studied about large time behavior, and Aiki and Sato [7] proved existence of periodic solutions.

On the other hand, numerical simulations have been only given in [4], in which Aiki, Murase, Sato and Shirakawa showed the following Figure 2 obtained by the numerical simulation.

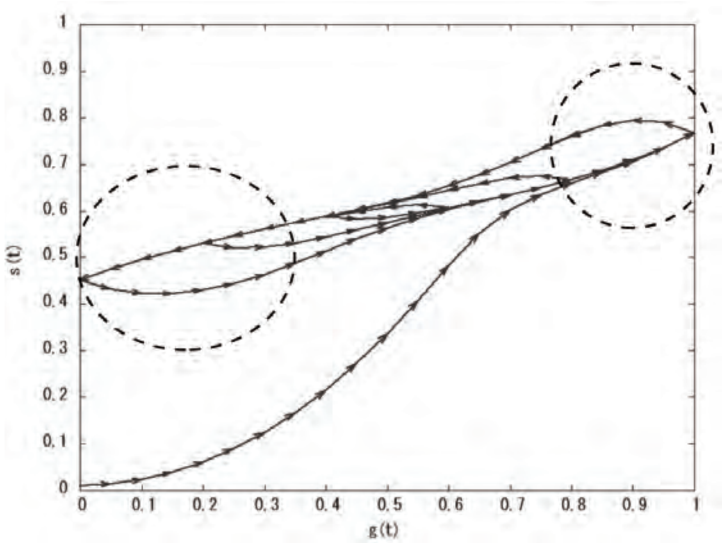

Figure 2: numerical simulation in [4]

Roughly speaking, the graphs in Figure 2 is almost same as that of Figure 1. Accordingly, we suppose that adsorption phenomena are represented by the model (S) to some extent. However, we find an issue on the simulation and a difference between Figures 1 and 2. The issue is that there exist few mathematical arguments on the numerical simulation to this system, since (S) is approximated by an experimental way in [4]. The difference between Figures 1 and 2 is observed as follows. In the real phenomena, the shape of graph is sharp when changing the process from wetting to drying, and from drying to wetting (see dotted circle area in Figure 1). On the other hand, the shape of the graph is a little bit swollen when changing the process (see dotted circle area in Figure 2). We guess that the mathematical system or our numerical way causes the difference of the graphs. In order to give an answer to this conjecture we try to simulate model (S) by a different way from that of [4]. Precisely, by applying the finite element method with the adaptive moving mesh method we obtain numerical solutions in the present paper. The adaptive moving method is a numerical technique redeciding mesh positions depending upon numerical solutions of the system at each time step, automatically. (For the detail, see [3], for example.)

In this paper, we propose a discretization scheme of (S) based on the finite element method with the adaptive moving mesh method in Section 2. In Section 3, we show our results of numerical simulations. Finally, we organize conclusions and future plans in Section 4.

2 Numerical approximation of model (S)

Let $Q = (0, T) \times (0, 1)$, and $\tilde{u}(t, x) = u(t, (1 - x)s(t) + Lx)$ for any $(t, x) \in Q$. By change of variables, the system (S) is transformed to the following system (AS):

$$\rho_v \tilde{u}_t(t, x) - \frac{\kappa}{(L - s(t))^2}\tilde{u}_{xx}(t, x) = \frac{\rho_v(1 - x)s'(t)}{L - s(t)}\tilde{u}_x(t, x) \quad \text{on } Q, \tag{7}$$

$$s'(t) = \alpha(s(t), \tilde{u}(t, 0)) \quad \text{for } 0 < t < T, \tag{8}$$

$$\tilde{u}(t, 1) = g(t) \quad \text{for } 0 < t < T, \tag{9}$$

$$\frac{\kappa}{L - s(t)}\tilde{u}_x(t, 0) = (\rho_w - \rho_v \tilde{u}(t, 0))s'(t) \quad \text{for } 0 < t < T, \tag{10}$$

$$\tilde{u}(0, x) = \tilde{u}_0(x) \quad \text{for } 0 < x < 1, \tag{11}$$

$$s(0) = s_{(0)}. \tag{12}$$

Moreover, we assume the following conditions (P1) to (P4) for our simulation.

(P1) Assume that it is able to present $x = x(t, \xi)$ satisfying

$$x(t, \xi_1) \neq x(t, \xi_2) \text{ for } \xi_1 \neq \xi_2 \text{ and every } t \in [0, T).$$

(P2) $N \in \mathbb{N}$, $\xi_n = \frac{n}{N}$ $(n = 0, 1, \cdots, N)$, and $x_n(t) = x(t, \xi_n)$ for every $t \in [0, T)$.

(P3) $\tau = \Delta t > 0$, and $t_m = m\tau$ for $m = 0, 1, \cdots$, where Δt is the size of the time mesh.

(P4) $\tilde{u}_{m,n} = \tilde{u}(t_m, x_n(t_m))$, $s_m = s(t_m)$ for all $n = 0, 1, \cdots, N$, $m = 0, 1, \cdots$.

Our discretization of the system (AS) consists of 5 steps. We present these steps under conditions (P1) to (P4).

Step 1. (Setting initial conditions)

From (12), (11), we put $\tilde{u}_{0,n} = \tilde{u}_0(x_n(0))$ for $n = 0, 1, \cdots, N$, the initial index $m = 1$, and $x_n(0) = \frac{n}{N}$ for $n = 0, 1, \cdots, N$. In this time, we adopt an equable mesh for the initial mesh position.

Step 2. (Deciding the position of the free boundary)

Descretizing (8) by the forward finite difference, and we decide next position of the free boundary by

$$s_m = s_{m-1} + \tau\alpha(s_{m-1}, \tilde{u}_{m-1,0}).$$

Step 3. (Deciding the position of the mesh)

Deciding next mesh position $x = x(t, \xi)$ by the following differential equation:

$$\frac{\partial x}{\partial t} = \frac{1}{\rho\beta} \cdot \frac{\partial}{\partial \xi}\left(\rho \frac{\partial x}{\partial \xi}\right) \text{ in } Q, \tag{13}$$

$$x(t, 0) = 0, x(t, 1) = 1 \text{ for any } t \in (0, T), \tag{14}$$

where $\beta > 0$, and

$$\rho := \rho(t, x) = \left\{1 + \frac{1}{\gamma(t)}|\tilde{u}_{xx}|^2\right\}^{\frac{1}{3}}, \quad \gamma := \gamma(t) = \max\left\{1, \left(\int_0^1 |\tilde{u}_{xx}|^{\frac{2}{3}} dx\right)^3\right\}.$$

We get next mesh positions $x_n(t_m)$ $(n = 0, 1, \cdots, N)$ by solving this equation with the finite difference method.

Step 4. (Deciding numerical solutions $\tilde{u}_{m,n}$ $(n = 0, 1, \cdots, N)$)

Applying the finite element method to (7) and solve the approximated equation, we decide numerical solutions $\tilde{u}_{m,n}$ $(n = 0, 1, \cdots, N)$.

Step 5. (Renewing time step)

Increment the value of m, and back to Step 2. We finish calculating when the step count reaches to the appointed value.

3 Numerical simulations

In our numerical simulation, conditions and parameters are same as in [4]. Details of values of the parameters are as follows.

$$L = 1, \quad \kappa = 1, \quad \rho_w = 1, \quad \rho_v = 1.73 \times 10^{-5}, \quad s_{(0)} = 0.01, \quad \beta = 0.01.$$

The initial function u_0 is

$$u_0(x) = 0 \text{ for } x \in (s_{(0)}, L),$$

the function $\alpha(\cdot,\cdot)$ is

$$\alpha(s,u) = (1+u^2)\left(u - \frac{\arctan(10s-6) - \arctan(-6)}{\arctan(4) - \arctan(-6)}\right),$$

and the boudary function g is

$$\text{and} \qquad g(t) = \begin{cases} \frac{t}{5} \ \text{ if } \ 0 \le t \le 5, \\ 2 - \frac{t}{5} \ \text{ if } \ 5 \le t \le 10, \\ \frac{t}{5} - 2 \ \text{ if } \ 10 \le t \le 15, \\ 4 - \frac{t}{5} \ \text{ if } \ 15 \le t \le 19, \\ \frac{t}{5} - 3.6 \ \text{ if } \ 19 \le t \le 22, \\ 5.2 - \frac{t}{5} \ \text{ if } \ 22 \le t \le 24, \\ \frac{t}{5} - 4.4 \ \text{ if } \ 24 \le t \le 25, \\ 5.6 - \frac{t}{5} \ \text{ if } \ 25 \le t \le 26. \end{cases}$$

Furthermore, we put $N = 20$, $\Delta t = 0.001$, and we decide to evenly arrangement the initial mesh position.

Under the conditions, we get the following results. Figure 3 is a graph of the relationship between $s(t)$ (saturation) and $g(t)$ (humidity) obtained in [4], and Figure 4 is that of our present result. From these pictures, we can see that two numerical solutions are almost same. It shows that not only the numerical result in [4] is a valid result, but also we can deduce swellings of the graph are not given by numerically discretization techniques, but given by the equations or parameters of the numerical simulations.

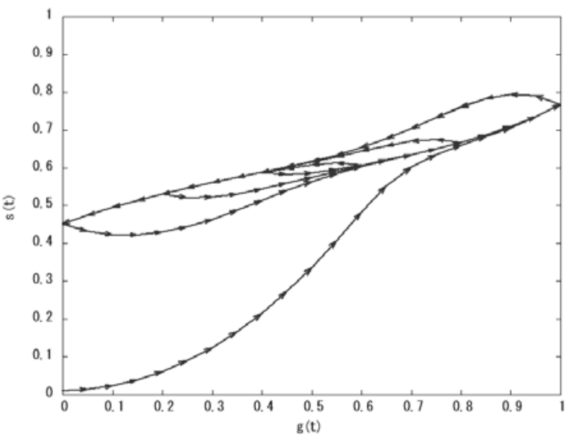

Figure 3: Result in [4]

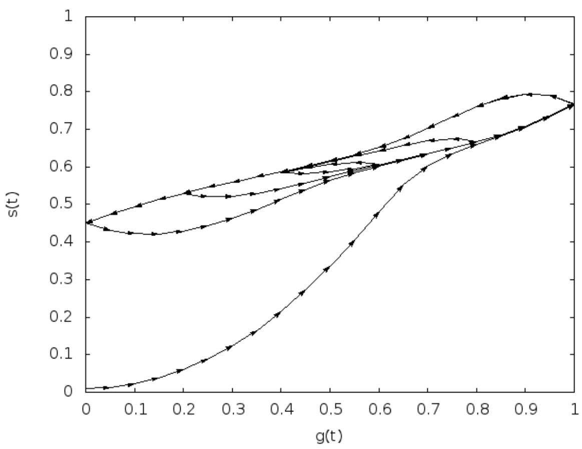

Figure 4: Our result

Figure 5 in the next page indicates the transitions of mesh positions obtained by the adaptive moving mesh method. As far as we observe the numerical result, by applying adaptive moving mesh method the mesh positions move little. Namely, the positions seem to be almost fixed.

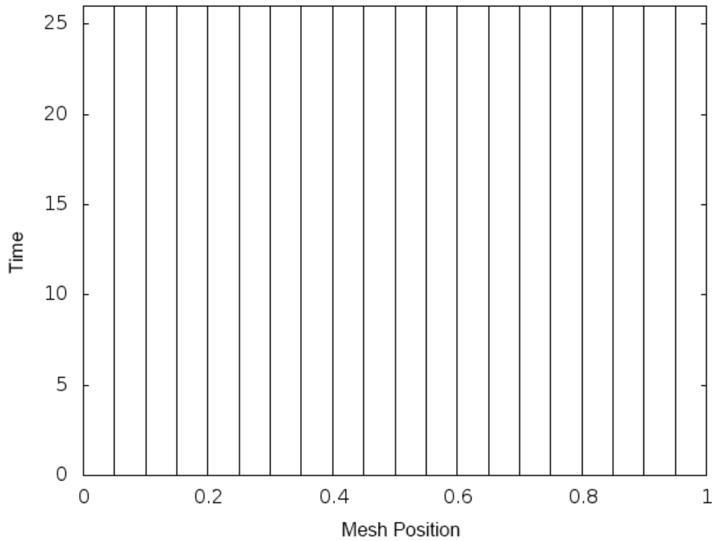

Figure 5: Mesh position change

4 conclusions and future problems

From our numerical simulations we ensure that the numerical results in [4] is valid, and we conjecture that the swelling of the graph of relationship between s and g does not come from our numerical techniques. Since some settings of our numerical simulation are not enough to fit to the real phenomena, we need to continue this investigation, more.

In addition, we have to prove solvability of our numerical procedure, numerical stability, error estimate, and convergence to solutions of system (S) in order to guarantee accuracy of our numerical simulation. In particular, we will discuss the solvability of the numerical scheme in our forthcoming paper [8].

References

[1] K. Maekawa, T. Ishida, T. Kishi, Multi-scale modeling of concrete performance, *Journal of Advanced Concrete Technology*, **1** (2003), 91 − 126.

[2] K. Maekawa, R. Chaube, T. Kishi, *Modeling of concrete performance*, Taylor and Francis, 1999.

[3] W. Huang, R. D. Russell, Adaptive Moving Mesh Methods, Springer, 2011.

[4] T. Aiki, Y. Murase, N. Sato, K. Shirakawa, A mathematical model for a hysteresis appearing in adsorption phenomena, *Sūrikaisekikenkyūsho Kōkyūroku*, **1856** (2013), 1-12.

[5] N. Sato, T. Aiki, Y. Murase, K. Shirakawa, A one dimensional free boundary problem for adsorption phenomena, *Netw. Heterog. Media* **9** (2014), no.4, 655-668.

[6] T. Aiki, Y. Murase, On a large time behavior of a solution to a one-dimensional free boundary problem for adsorption phenomena, *J. Math. Anal. Appl.* **445** (2017), no.1, 837-854.

[7] T. Aiki, N. Sato, Existence of periodic solution to one dimensional free boudary problems for adsorption phenomena, *Izv. Irkutsk. Gos. Univ. Ser. Mat.* **25** (2018), 3-18.

[8] T. Kishida, Y. Murase, Solvability of numerical scheme for water adsorption model generated by finite element method with adaptive moving mesh method, *in preparation.*