Proceedings of the Fifth IIEEJ International Workshop
on Image Electronics and Visual Computing 2017
Da Nang, Vietnam, February 28- March 3, 2017

Modeling and Simulation of Rust Based on Chemical Reaction Processes

Tomokazu Ishikawa[*†] *Yusuke Kameda*[*] *Masanori Kakimoto*[‡†] *Ichiro Matsuda*[*] *Susumu Itoh*[*]

[*]Tokyo University of Science [†]UEI Research [‡]Tokyo University of Technology

ABSTRACT

Secular change is an important factor in order to produce realistic computer graphics (CG) images; rust that generates on metal is one example of secular change. The appearance of rust depends on the type of metal, adherence of water by rain or sea water, the quantity of dissolved oxygen in water, and effects of running water; to our knowledge, there are no simulation models of rust that take into account the chemical reaction processes of rust. In the proposed method, we performed a fluid simulation, calculated the adherence and flow of water using 3-dimensional models, and calculated the progression of corrosion from the site of adherence. This corrosion simulation took into account conditions such as the quantity of adherence and the chemical reaction process. As a result, we confirmed that the mass loss of metal was near to the theoretical value and that CG images were similar to those of actual rust.

1. CHEMICAL REACTION PROCESSES OF RUST

Rust is a corrosion phenomenon and is generated as a result of metal corroding. There are two types of metal corrosion, namely, "wet corrosion" and "dry corrosion." When metal corrodes with oxygen and water, it is known as wet corrosion, and when metal is exposed to high temperatures in gases such as air or to some chemicals, it is known as dry corrosion. This study focuses on the wet corrosion that can be observed in our daily lives.

Rust differs in its colors depending on the type of metal. The corrosion that is ordinarily called rust is the red rust that occurs on steel. Green copper rust is commonly seen on bronze statues, and white rust occurs on zinc and aluminum. We focus on red rust, which is known as ordinary rust. As an experiment, we poured water onto a steel plate to observe the formation of rust (Figure 1).

$$\mathrm{Fe} \rightarrow \mathrm{Fe}^{2+} + 2e^{-} \quad (1)$$

$$2\mathrm{H}^{+} + 2e^{-} \rightarrow \mathrm{H}_2 \quad (2)$$

$$2\mathrm{H_2O} + 2e^{-} \rightarrow 2\mathrm{OH}^{-} + \mathrm{H}_2 \quad (3)$$

$$\mathrm{O}_2 + 2\mathrm{H_2O} + 4e^{-} \rightarrow 4\mathrm{OH}^{-} \quad (4)$$

$$\mathrm{Fe}^{2+} + 2\mathrm{OH}^{-} \rightarrow \mathrm{Fe(OH)}_2 \quad (5)$$

Fig. 1: Rust generated by flowing water. (45 min.)

$$\mathrm{Fe(OH)}_2 + \frac{1}{4}\mathrm{O}_2 + \frac{1}{2}\mathrm{H_2O} \rightarrow \mathrm{Fe(OH)}_3 \quad (6)$$

Formula (1) expresses the oxidizing reaction of steel, which produces electrons, as water adheres to steel. Formulae (2) – (4) express the reduction reaction of the water, which receives the electrons produced by the steel. It is known that the steel surface locally becomes an electric cell, and this is the cause of corrosion. The reaction rate at which the steel changes to ferric ion can be calculated by the amount of current. This study includes the formula for calculating the steel reduction caused by these reaction processes. Formula (5) addresses the formation of ferric hydroxide, which is the source of the red rust. This study calculates the formulation of ferric hydroxide by considering the speed of this reaction. Formula (6) expresses the chemical reaction of ferric hydroxide reacting to dissolved oxygen to produce ferric hydroxide. This study calculates the amount of red rust sediment by considering the amount of dissolved oxygen.

2. RELATED WORK

Chang et al. simulated the progression of rust in sea water [2]. To obtain a physical quantity for each polygon vertex in a 3D model, the physical quantity was updated by an L-System. This approach is an extension of the rust simulation method of Dorsey et al. [3]. In addition, the rust sets the progression level at a threshold of the production of cracking or perforation that can be caused by rust.

Kanazawa et al. [1] extended the study of Tanabe et al. [4], which used cellular automata to calculate the progression of rust considering the shape of an object, such as its tilt angle. In Tanabe's method, the probability

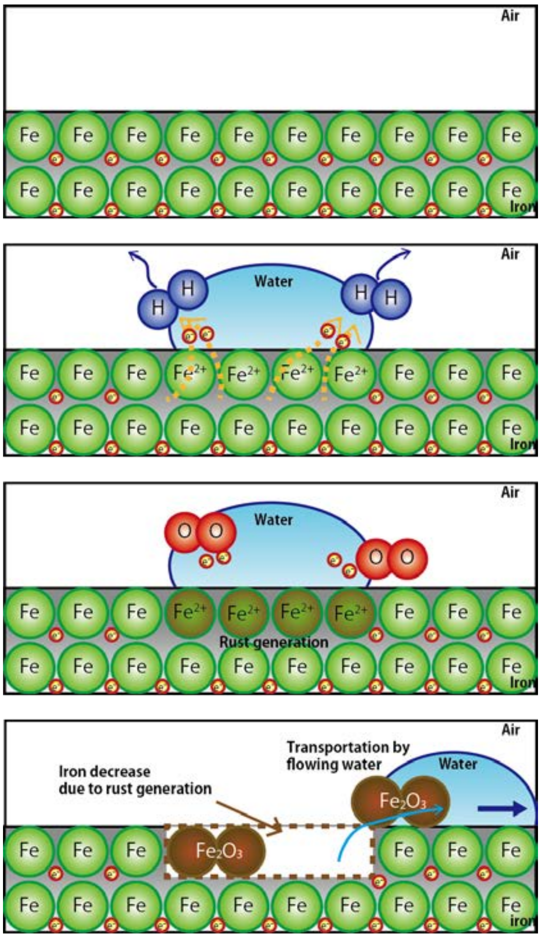


Fig. 2: Pattern diagram of rust generation process.

that rust will occur in each cell, expansion level, and color level parameters are given. When a cell rusts, it affects the existence of cells surrounding it, and by sufficiently increasing the resolution of the model, the progress of the rust tilt angle can be considered by weighting the value of a given angle in the direction of gravity.

A problem in research related to rust is that a chemical and physical basis has not been used to generate rust progression. For that reason, these simulation results are ambiguous as to how much time has elapsed. Although the surface of iron becomes uneven, which because of the decrease in iron and deposits of rust, this is not taken into consideration in the model and irregularities cannot be expressed. Because the rust color varies due to this unevenness, not only is the color visually important, but it also leads to a technique to calculate at the unevenness in the proposed method.

Tanaka et al. performed an aging study that takes into account the adhesion of water [5], and there is a study of landscape changes due to water contamination by Dorsey et al. [6]. In these studies, dirt is represented as particles. Some dirt particles are taken by particles of water flowing over the model's surface, depositing a portion of the soil within the particle of water. By adopting the transportation and sedimentation caused by water particles, the flow of rust is represented as water in the proposed method.

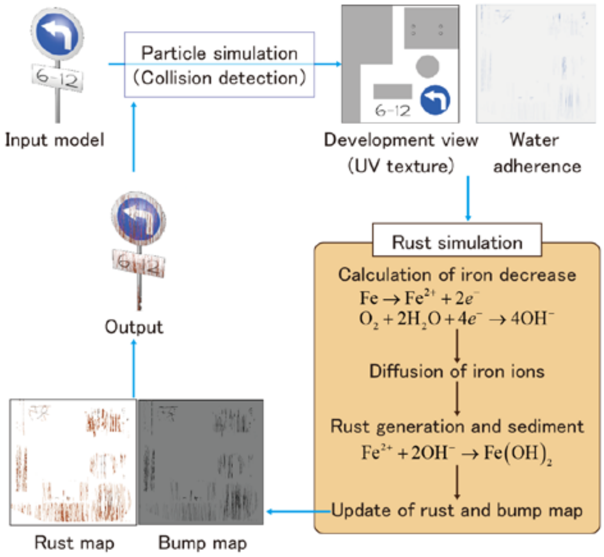


Fig. 3: Flow of the proposed method.

3. OUR METHOD

In this section, we explain the proposed method for a modeling and simulation of rust generation.

3.1. Processing Flow

A block diagram of our proposed method is shown in Figure 3. The input to the proposed system is a 3D model and its UV development diagram. We position the 3D model in air, simulate the particles, and add the positions of particles in the 3D model as water attachment information to the part of the UV development diagram the particles will hit according to their mesh positions. We next perform a rust simulation on the surface of the 3D model (the UV development diagram) based on the water attachment positions. Taking into account the chemical reaction in this rust simulation, we calculate the amount of rust and the roughness caused by the corrosion of metal, and then output both as a texture. By applying these textures to the 3D model, we can express the generation and progress of the rust.

In our proposed method, we judge the collisions with the 3D model using SPH after the advection of the particles. We attach a certain amount of water to the model surface within an effective radius area where the collision was judged to occur. The amount of adhesion is stored in pixel units in the UV development diagram. The adhesion amount of water represents the thickness of water at each pixel. We set an upper limit of the thickness and perform an additional processing up to this upper limit when the adhesion progresses at the same coordinates. In addition, we periodically decrease this thickness to simulate the effect of water evaporation. The particles carry and deposit rust and water on the surface. To simulate this phenomenon, we adopt the flow model that was proposed by Dorsey et al. [3].

We calculate the external forces in the SPH method using a penalty method, including a normal force that occurs at the time of collision with the model, and also calculate the surface tension between the surface of the model and the particles.

3.2. Rust Simulation

The production of rust is calculated using the amount of adhesion of water calculated in the previous section. Because the transportation and sedimentation of water was discussed in the previous section, calculations for still water are discussed here. The speed of the corrosion reaction can be determined from the current flowing at the time of the oxidation-reduction reaction. Here the steps in this process are shown in Figure 3. The calculation is carried out on the texture of the model's surface and the physical quantity is stored in pixels. The dissolved oxygen concentration in water is calculated from the adhesion of the water to the 3D model, which is obtained from the fluid calculation. The dissolved oxygen concentration will be higher if the amount of water adhesion increases. This assumption follows the first law of Fick, which says that when the concentration of a chemical is not uniform, it will diffuse in proportion so as to equalize the concentration. Therefore, in the proposed method, the dissolved oxygen concentration near the iron surface is zero because of the oxidation process, the concentration at the surface between the water and atmosphere is the highest, and the concentration increases in proportion to the distance from the iron surface to the diffusion layer.

Iron is ionized when water and oxygen make contact with it. The lost mass ΔW calculated by Equation (7) is used in Equation (9) to calculate the amount of reduction ΔH of the thickness of the iron.

$$\Delta W = \frac{MIS\Delta t}{\alpha F}, \tag{7}$$

$$I = \frac{\beta FDC}{\delta}, \tag{8}$$

$$\Delta H = \frac{\Delta W}{\rho S}, \tag{9}$$

where M is the atomic weight of iron, I is amperage, S is surface area, ΔH is transit time, α is a charge number of iron, F is the Faraday constant, β is a charge number of oxygen, D is a diffusion constant of dissolved oxygen, C is dissolved oxygen level, δ is thickness of diffusion layer, and ρ is density of iron.

The lost mass indicates the amount of iron lost from the surface, which should be the same as the amount of iron ions dissolved in the water. The iron ions dissolved in the water diffuse from the vicinity of the iron surface to the areas of the water with lower concentration. This diffusion follows the diffusion equation. Diffusion is calculated only for the volumes occupied by water. For volumes where water does not exist, a Dirichlet boundary condition is adopted.

$$\frac{\partial[\mathrm{Fe}^{2+}]}{\partial t} = D_{\mathrm{Fe}}\nabla^2 \frac{\partial^2[\mathrm{Fe}^{2+}]}{\partial \mathbf{x}^2}, \tag{10}$$

where [X] shows concentration of X and D_{Fe} is a diffusion constant of iron ions.

Finally, the rate of ferrous hydroxide production is determined. The reaction rate of Formula (5) is calculated using Equation (11). By setting the water temperature and pH, a constant concentration of hydroxide ions in water is determined. Next, the red rust production rate in Formula (6) is calculated using Equation (12).

$$\frac{\Delta[\mathrm{Fe(OH)}_2]}{\Delta t} = k_1[\mathrm{Fe}^{2+}][\mathrm{OH}^-]^3, \tag{11}$$

$$\frac{\Delta[\mathrm{Fe(OH)}_3]}{\Delta t} = k_2[\mathrm{Fe(OH)}_2]^m[\mathrm{O}_2]^n, \tag{12}$$

where k_1 is a rate constant of reaction on Formula (5) and k_2 is a rate constant of reaction on Formula (6).

Because ferrous hydroxide (III) is insoluble in water, the amount produced immediately becomes the amount of sediment in the water. This amount can be determined by multiplying the concentration per pixel with the unit volume.

In order to present the simulation results, unevenness data and a color table indicating the amount of rust sediment are presented. The color and unevenness are successively updated in accordance with the reduction in iron thickness in Equation (9) and the amount of rust sediment in Equation (11). A darker color is used for places with more rust sediment, and the surface appears uneven because the unevenness data is mapped as bumps on the surface.

4. RESULTS AND CONCLUSION

The changes in appearance and reduction of thickness were calculated and compared with the theoretical values to verify the proposed rust simulation model. The theoretical value for the corrosion reaction rate for water adhesion is 0.2 mm/y, and the simulation result is 0.192 mm/y, which indicates that the reduction in iron thickness caused by corrosion is sucessfully reproduced. Figure 4 compares the simulation results using this method with the theoretical value for thickness reduction over time [8].

Figure 5 compares the results of simulation using this method, that of a previous method using cellular automata, and the rust of an actual iron plate. Figure 5(b) shows the simulation results obtained by the previous method using the same water adhesion information. By comparing Figures 5(a) and (b) with the picture of rusted iron, it is clear that the thickness of water as a result of simulation using this method is as thin as the actual images, and there is more rust at places with higher dissolved oxygen concentration (near the boundary between water and atmosphere). Hence, taking water adhesion into consideration is effective.

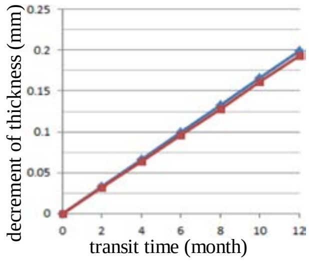
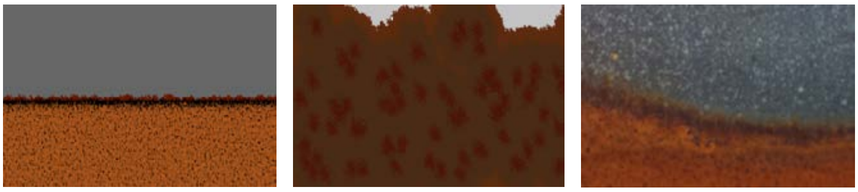
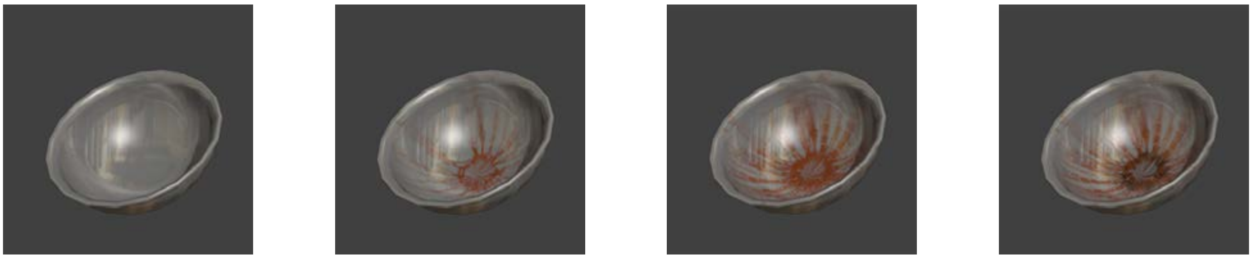


Fig. 4: Comparison with the theoretical value (blue line) and simulation result (red line).



(a) Proposed method (b) Cell automaton [1] (c) Photograph

Fig. 5: Comparison with related work.



(a) Original model (b) 200 timesteps (c) 400 timesteps (d) 600 timesteps

Fig. 6: Result images (bowl).

(a) Photograph (45min.) (c) Simulation (4500 timestep)

(b) Photograph (75min.) (d) Simulation (7500 timestep)

Fig. 7: Simulation result of rust generation by water flow.

In addition, the variation of unevenness due to the corrosion process can also be expressed in this method as height information.

Figure 6 shows the results of simulating the state of rust production due to water falling from above in a bowl model (Figure 6(a)). Figures 6(c) and (d) show the results of simulation after further adding in water based on the results of Figure 6(b). Water drops falling in the direction of gravity adhere, and rust occurs along the flow of water. In addition, the model also reproduces the fact that the rate of corrosion is faster in the places water tends to accumulate.

Figure 7 shows the result of simulating the transportation and sedimentation of rust due to water flow. It shows that the amount of sediment is smaller in places with strong water flow, as the rust is washed away. In contrast, the corrosion progresses in areas with weaker water flow.

We were able to simulate rust in 3-dimensional space by coating the model with water in 3-dimensional space by the proposed method for forming rust. In addition, we were able to reproduce the rust more realistically because a detailed parameter was used. This research targeted rust simulation only. However, we believe that it would be able to handle various metals such as copper rust and the white rust formed on aluminum if we change the chemical reaction process.

REFERENCES

[1] K. Kanazawa, R. Tanabe, T. Moriya, T. Takahashi: Rust-Aging Simulation Considering Object's Geometries, SIGGRAPH 2015 Posters (2015).

[2] Y. Chang, Z. Shin: The synthesis of rust in seawater, The Visual Computer, Vol. 19, No. 1 pp.50-66, 2003.

[3] J. Dorsey, P. Hanrahan: Modeling and Rendering of Metallic Patinas, SIGGRAPH 1996, pp.387-396, 1996.

[4] R. Tanabe, T. Moriya, T. Takahashi: A Generation Method of Rust Aging Texture, IEICE General Conference, 2013 (in Japanese).

[5] M. Tanaka, K. Tokoi: GPU Acceleration of Particle Method Simulation of Rain Stains, The journal of The Society for Art and Science, Vol. 12, No. 3, pp. 124-131 2013 (in Japanese).

[6] J. Dorsey, H. K. Pedersen, P. Hanrahan: Flow and Changes in Appearance, SIGGRAPH 2005, pp.411-420, 2005.

[7] B. Case: The diffusivity of oxygen in dilute alkaline solution from 0° to 65°C, Electrochimica Acta., Vol. 18, Issue 4, pp.293-299, 1973.