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Numerical Study of Random Corrosion Characteristics of Metal Based On the Cellular Automata Method

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Abstract: In the production process of coal chemical companies, the corrosion of metal equipment and the resulting shortening of its service life can cause safety hazards. Simulation modeling of pit emergence and development during corrosion evolution provides a new approach to corrosion research. By analyzing the effect of different parameters on causing corrosion to occur, it is possible to reflect the influence of complex physico-chemical systems. In this paper, the simulation of a meta-cellular automaton model of pit growth under diffusion and the introduction of a passivation probability to correct the chemical reaction rate are developed; The effect of reaction passivation probability, chemical reaction rate and diffusion coefficient on the degree of corrosion was also analyzed by means of quantitative analysis. The results show that for metal corrosion loss processes, the degree of corrosion damage decreases with increasing probability of reactive passivation and increases with increasing chemical reaction rate, increasing electrolyte concentration and increasing time step. The CA model was applied to simulate the growth and change of pitting corrosion of metal materials with their corrosion protection layer under damaged conditions. The corrosion model can simulate the corrosion morphology change characteristics similar to the real metal to the corrosion pit evolution simulation related research has certain scientific, validity, reference.

Keywords: Metal pitting simulation, electrochemical reaction, cellular automata method, numerical simulation

1. Introduction

Corrosion evolution modeling will simultaneously involve multi-phase problems, multi-dimensional problems, and the coupling between different physicochemical phenomena such as particle diffusion, electrochemical reactions, etc., in which the change of the elements in the corrosion process and the generation of corrosion products involves the influence of complex physical and chemical factors, some of which cannot be accurately described and have a random nature.

Before the emergence of CA numerical simulation, the main focus of research is the electrochemical and chemical aspects of corrosion. In the actual industrial production is often a variety of corrosion types mixed occurrence, interaction, and artificially accelerated corrosion experiments are more complex to implement, not only can not the real-time observation of the process of the emergence and development of corrosion pits but also cannot be in-depth to figure out the mechanism of corrosion occurrence. The numerical simulation study of corrosion using relevant mathematical models can, to a certain extent, make up for the shortcomings of traditional methods.

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Early on Meakin [1] used the CA model to carry out a simulation study of the evolution of crater morphology and to develop a two-dimensional passivation and depassivation model for pitting. He Le Ru et al [2] used a 2D CA model to simulate the evolution of corrosion pits over time and observed different pitting shapes by adjusting the relevant parameters. Bartosik et al [3] studied corrosion damage and passivation on the surface of metallic materials in depth using cellular automata Chen Mengcheng et al [4] simulated the electrochemical reactions and diffusion processes during metal corrosion defining local evolution rules for the meta-cellular automata model, but the simulations produced pit morphologies that differed from reality.

Although there have been several research results using meta-cellular automata to simulate the evolution of metal corrosion damage, due to the different corrosion mechanisms, the existing results usually focus on the evolution of metal corrosion pits in specific situations, and there are relatively few studies on the accelerating effect of various parameters on the steel corrosion process in a corrosive environment.

In this paper, the influence of the pitting corrosion evolution process on the surface morphology of the specimen is modeled using a cellular automaton with stainless steel as the research object. The material transfer, metal dissolution and passivation processes in the metal corrosion process are simulated to investigate the effects of parameters such as electrolyte concentration, dissolution probability, and passivation probability on the evolution process of corrosion damage on the surface and depth direction of individual pits. To provide theoretical guidance and experimental reference for the safe service and design guidelines of metal equipment in coal chemical enterprises.

2. Model

Since the corrosion process is a complex process involving the influence of physical and chemical factors, some of which cannot be accurately described and are stochastic in nature, it is difficult to describe its evolution by solving the partial differential equation alone.

The essence of the electrochemical corrosion process on the metal surface is that it constitutes an electrochemical corrosion cell, in which an oxidation reaction occurs at the anode to produce metal ions and electrons; a reduction reaction occurs at the cathode to consume the electrons produced at the anode. The corrosion process can be defined as two processes of dissolution and passivation, respectively, according to the process can be defined CA model reaction rules as shown in Fig. 1.

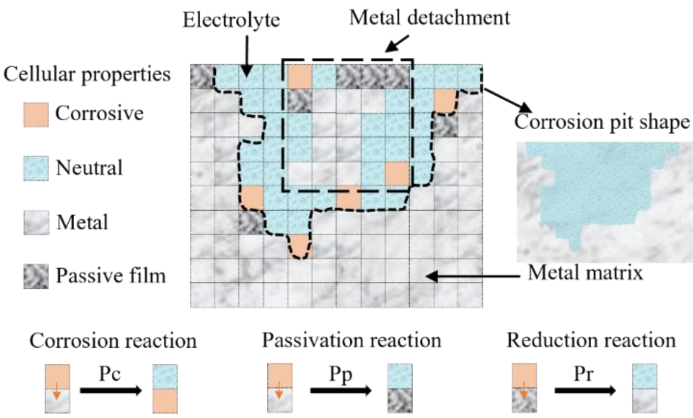

Fig. 1 - Evolutionary rules for simulation of corrosion damage by cellular automata

Due to the autocatalytic effect of the occluded corrosion cell leads to a non-uniform medium in the hole, so the corrosion rate in the corrosion pit is characterized by spatial non-uniformity. In the evolution model, besides the pit initiation model and the pit growth model, the growth process of pits is also affected by other parameters [5]. Among these parameters, the difference of the corrosive environment has a great influence on the probability of corrosion reaction Pc, the probability of passivation reaction Pp and the concentration of corrosive medium c. The control variable method was used to explore the influence of different parameters in the CA model on the evolution process of the erosion pit. The initial variables of the model are simplified through the definition of key parameters to reflect the change of external conditions and the randomness of pit growth. According to the set evolution rules, it simulates the global evolution process of a specific dynamic system along the time dimension in the planned neighborhood space, and has the characteristics of locality, homogeneity, parallelism and so on [6].

In order to fully describe the geometric size of the corrosion pit, the surface damage degree α is introduced to describe the damage morphology of the metal surface, and α(t) is a function of time [7]:

$$\alpha(\mathrm{t}) = \frac{N_{\mathrm{Corr}}(t)}{\left(Nx \times \left(1 - \frac{Ny}{w}\right)\right)} \times 100\% \quad (1)$$

Along the length and width directions of the metal surface, the number of metal cells M is represented by $(Nx\times(1-Ny/w))$, where 1/w is the proportion of the electrolyte layer to the overall number of layers in the model, Assuming that there are n corrosion pits on the metal surface during the simulation time 0-t, Ncorr(t) represents the total number of metal cells corroded in the n corrosion pits on the metal surface during the period of 0-t. Ncorr(t), Nx and Ny are dimensionless quantities.

The CA model implementation process is shown in Fig. 2:

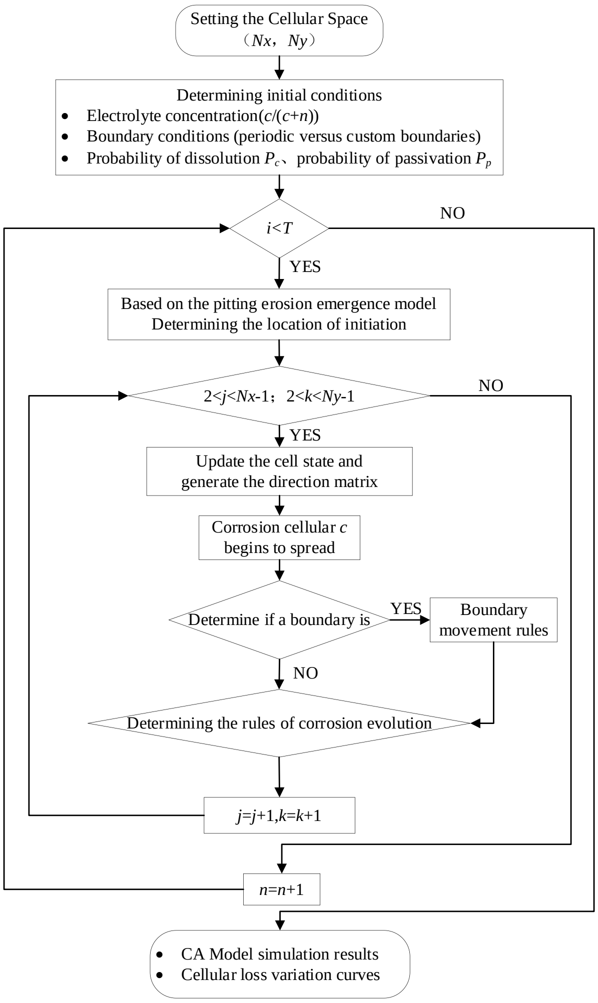

Fig. 2 - CA corrosion model and evolution rules

3. Results and Discussion

Fig. 3 shows the shape of the pitting pits on the metal surface as a function of time. It can be seen from the figure that the corrosion degree of the damaged part gradually deepens with the change of time. Due to the influence of the passivation probability, the shape of the corrosion pit also changes randomly and irregularly [8].

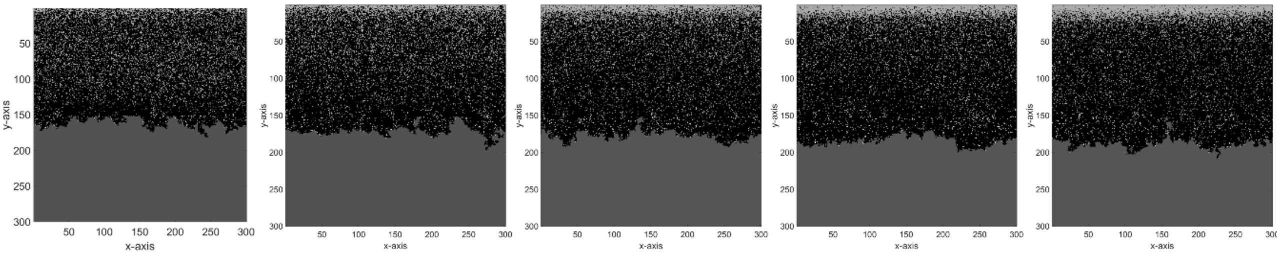

Fig. 3 - Comparison of uniform corrosion morphology of metal substrate surface in electrolyte under different time periods

It can be seen from the instantaneous image of the model that with the increase of the simulation time, the corrosion loss of the metal surface increases rapidly, and then tends to be stable, and the cell loss gradually increases. The relationship between the two is shown in Fig. 4.

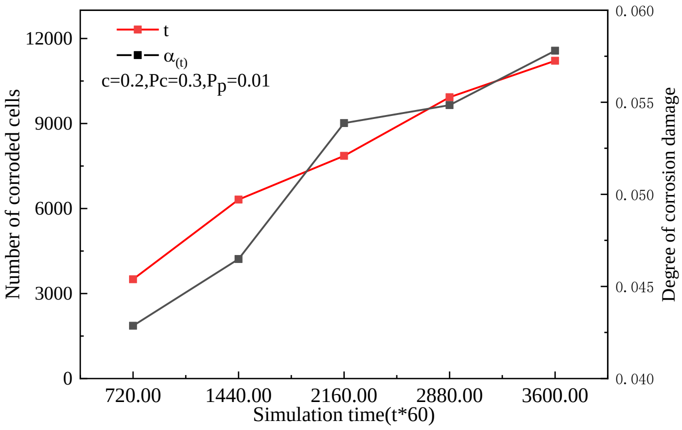

Fig. 4 - Changes in the number of corroded cells and the degree of damage under different time periods

Due to the non-uniformity of the medium in the pores due to the autocatalysis of the occluded corrosion cell, the corrosion rate in the corrosion pit is characterized by spatial non-uniformity. The increase of the passivation probability Pp will lead to the gradual decrease of the corrosion rate and the gradual reduction of the corrosion degree. The trend is shown in Fig. 5.

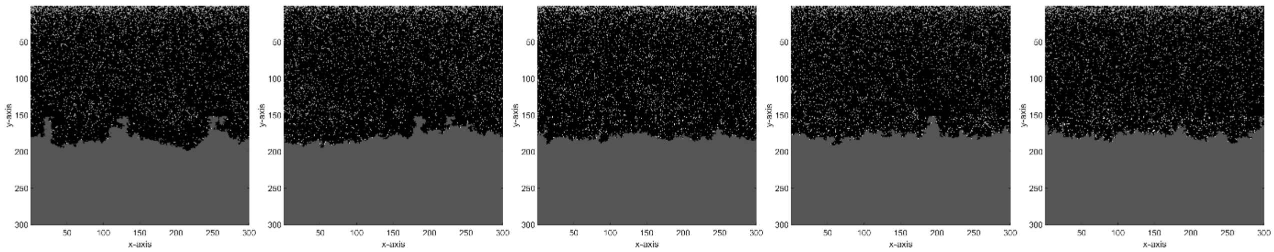

Fig. 5 - Comparison of uniform corrosion morphology of metal substrate surface in electrolyte under different passivation probabilities

With the increase of the passivation probability Pp, the number of passivated metal cells gradually increases, which is reflected here as the passivated metal covering the metal surface hinders the further development of corrosion, so that the corrosion rate gradually decreases, and the depth of the corrosion pit develops. slow down. The relationship between the passivation probability and the number of corroded cells is shown in Fig. 6.

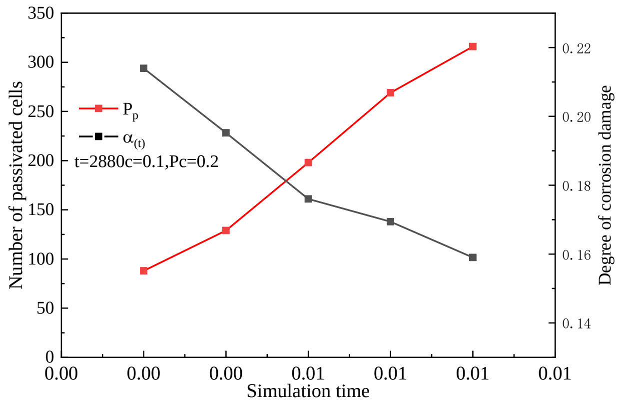

Fig. 6 - Variation of the number of corroded cells and the degree of damage under different passivation probabilities

In the metal adsorption theory, it is believed that when the metal surface adsorbs molecules, it will produce a good passivation film effect, and the molecular adsorption amount can only be the number of single-layer molecules at most, and it is generally believed that the adsorption will be oxygen atoms. [9]. When the oxygen atoms and the metal outer layer atoms are adsorbed and combined together, the chemical bonding force on the metal surface will be saturated, which will lead to the change of the interface structure between the metal and the solution, which will increase the activation energy of the anodic reaction of the metal and slow down the corrosion rate of the metal [10]. It shows that it is feasible to use the CA model to simulate the metal corrosion process in actual working conditions.

It can be seen from Figs. 7 and 8 that the loss of metal cells has a linear relationship with the simulation time. As the corrosion progresses, the number of dissolved metal cells has a trend of increasing gradually with the simulation time. In addition, the increase of electrolyte concentration and the increase of corrosion probability led to serious corrosion damage area on the metal surface.

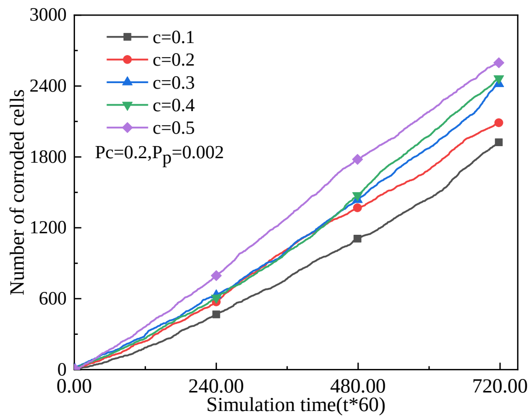

Fig. 7 - The uniform corrosion loss trend of metal substrate surface in electrolytes with different concentrations

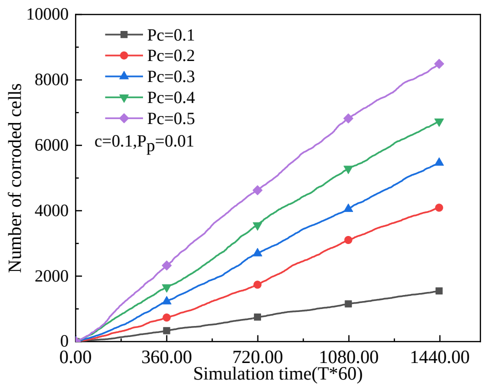

Fig. 8 - Uniform corrosion loss trend of metal substrate surface in electrolyte under different corrosion probabilities

This is because the initial position of the corrosion pit has been determined. Under the same parameters and step size, the increase of the concentration and corrosion probability Pc will lead to easier exchange of corrosive substances in the electrolyte solution. Corrosion occurs on the metal surface in direct contact with the electrolyte. The probability is higher, as the surface damage area increases, the number of corrosion cells entering the pit cavity increases.

4. Conclusion

The growth and changes of pitting corrosion of metallic materials and their anticorrosive layers under damage conditions were simulated using cellular automata, and a model of corrosion pit growth and diffusion under the influence of the corrosion pit growth model was established, while the effects of reaction passivation probability, chemical reaction rate, and diffusion coefficient on the degree of corrosion were analyzed by means of quantitative analysis. Using this corrosion model, the corrosion morphological change characteristics similar to those of real metals can be simulated.

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