

Review

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Review

# Cellular Automata Modeling as Tool in the Corrosion Management

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Abstract: Cellular automata (CA) models have emerged as a valuable tool in corrosion management. This manuscript provides an overview of the application of cellular automata models in corrosion research, highlighting their benefits and contributions to understanding the complex nature of corrosion processes. Cellular automata models offer a computational approach to simulate corrosion behavior at the microscale, capturing the intricate interactions between electrochemical reactions, material properties, and environmental factors generating a new vision of predictive maintenance. It discusses the key features of cellular automata, such as the grid-based representation of the material surface, the definition of state variables, and the rules governing cell-state transitions. The ability to model local interactions and emergent global behavior makes cellular automata particularly suitable for simulating corrosion processes. Finally, cellular automata models offer a powerful and versatile approach to studying corrosion processes, expanding models that can continue to enhance our understanding of corrosion and contribute to the development of effective corrosion prevention and control strategies.

**Keywords:** cellular automata; corrosion management; simulation corrosion; and modeling corrosion

#### 1. Introduction

Corrosion refers to the irreversible reaction between a material and its environment, which can result in the degradation of the material and its properties. It is a natural process that occurs when a metal is exposed to oxygen and moisture [1]. It has a significant economic impact, representing approximately 3.4% of the global Gross Domestic Product (GDP) [2]. Moreover, corrosion can lead to disruptions in activities and decrease the efficiency and productivity of affected industries. While catastrophic failures due to corrosion have not been reported in solar thermal power plants, there are potential risks. For example, the Fukushima nuclear plant accident prompted the search for alloys that can withstand extreme operating conditions [3]. In the case of solar thermal power plants with thermal energy storage systems (TES), various corrosion mechanisms can occur, such as intergranular corrosion and mechanically assisted corrosion [4].

Cellular automata are computational models used to study the behavior of complex systems by simulating their evolution over time. Consist of a regular grid of cells, each of which can exist in a finite number of states and interact with its neighboring cells according to a set of rules. These rules govern the transition of cells from one state to another and can be based on simple local interactions or more complex global behaviors. The concept of cellular automata was first introduced by mathematician John von Neumann in 1940 [5], but it was cellular automaton pioneer John Conway

popularized the idea in 1970. This manuscript recollects the main information about cellular automata models applied in corrosion management as an interesting tool for control and/or predictive maintenance of different types of corrosion, and factors that contribute to corrosion.

# 2. Cellular Automata as Tools in Corrosion Management.

Corrosion management refers to the systematic approach of preventing, controlling, and mitigating the effects of corrosion on materials and structures. It involves implementing strategies and practices to minimize the impact of corrosion, extend the service life, warrant safety, and reduce the maintenance and replacement of pieces or parts. Effective corrosion management includes preventive measures such as using corrosion-resistant materials, applying protective coatings or inhibitors, and proper new designs and considerations for regular inspection and maintenance. Corrosion management entails the proactive implementation of preventive measures, conducting regular inspections, performing thorough risk assessments, selecting appropriate materials, designing and constructing structures to minimize corrosion exposure, and employing a range of protective techniques, including coatings, corrosion inhibitors, cathodic protection systems, and other advanced technologies.

To effectively manage corrosion, a comprehensive understanding of the corrosion mechanisms associated with Hydrogen Evolution Reaction (HER), Oxygen Reduction Reaction (ORR), and Oxygen Evolution Reaction (OER) is crucial, along with a deep knowledge of the operating environment and the factors that can either accelerate or mitigate corrosion. Additionally, it is essential to consider the applicable regulations and safety standards from NACE [6] or another standard that can apply, pertaining to corrosion prevention across various industrial sectors, including petrochemicals [7], aeronautics [8], shipbuilding and maritime infrastructure [9–12], energy [13], mining [14], nuclear waste [15], microbial induced corrosion (MIC) [16], atmospheric corrosion [17], and among others. By incorporating this knowledge, industries can develop robust corrosion management strategies that ensure the safety, longevity, and optimal performance of their assets and infrastructure.

In the realm of corrosion management, the integration of computational techniques [18] and mathematical models [19] has emerged as an invaluable approach for comprehending and efficiently tackling the intricate behavior of corrosion processes. Among the array of techniques available, three stand out as particularly beneficial: cellular automata [20], Poisson processes [21], and Monte Carlo methods [22–25]. By harnessing these computational tools, researchers and engineers gain access to distinctive perspectives and capabilities, empowering them to simulate, analyze, and predict corrosion phenomena with remarkable precision and dependability.

The typical model such as Cellular Automata, Monte Carlo model, and Poisson processes are mathematical models that can be utilized in different aspects of corrosion management. In the field of corrosion, cellular automata have proven valuable information on the behavior of corrosion metals and alloys in contact with aggressive environments [26,27]. The cellular automata models generate interactions between electrochemical reactions, mechanical stresses, and material degradation, providing insights into the initiation, propagation, and evolution of various types of corrosion. Cellular Automata models considering the impact of environmental factors, in the optimization of corrosion-resistant materials.

Cellular automata models have proven to be valuable tools in corrosion management and mitigation strategies. They offer a computational framework for simulating and understanding the complex behavior of corrosion processes [28], enabling researchers and engineers to develop effective corrosion management techniques. The key applications of CA models in corrosion management are (i) predicting corrosion propagation, due which can simulate the propagation of corrosion in metallic structures, such as pipelines, bridges, or storage tanks [29]. These models can predict the spatial and temporal evolution of corrosion damage and help in identifying critical areas with corrosion and planning targeted inspection and maintenance activities [30], (ii) CA helps to understand the factors contributing to corrosion initiation, propagation, and the formation of localized corrosion features such as pits and crevices [31], (iii) CA can also be used to optimize corrosion management strategies

by exploring different scenarios [32] and decision-making processes. These models can evaluate the cost-effectiveness of various corrosion control measures, optimize inspection and maintenance schedules, and assess the long-term performance and durability of materials under different environmental conditions, (iv) CA the assessment of corrosion-related risks in different scenarios, considering environmental parameters, material properties, and corrosion rules, these models can estimate the probability and severity of corrosion-induced failures, allowing for better risk mitigation and resource allocation [33], (v) and CA can serve as educational tools to enhance the understanding of corrosion processes among students and professionals in the field, due visualizing corrosion behavior and the effects of different factors [34], these models facilitate learning and provide a platform for exploring corrosion management strategies.

By utilizing Cellular Automata models in corrosion management, researchers and engineers can gain valuable insights into corrosion processes, optimize corrosion control measures, and develop proactive strategies to mitigate the detrimental effects of corrosion.

# 2.1. Fundamentals of Cellular Automata for Corrosion.

The AC model was initially proposed by John Von Neumann and corresponds to an idealization of a physical system where time and space are discrete and physical quantities take on a finite set of values [5]. Space is represented on a grid of cells, and each cell has a specific state. In a simplistic way, the state of a cell can be assigned as either alive or dead (0 and 1), indicating its characteristic.

To clarify, for an entity to be classified as a CA (Counter Argument), it must adhere to the following structure. A regular grid of cells that covers a part of a d-dimensional space.

A set  $\Phi(\vec{r}, t) = {\Phi_1(\vec{r}, t), \Phi_2(\vec{r}, t), ..., \Phi_m(\vec{r}, t)}$  of Boolean variables attached to each site r of the grid that gives the local state of each cell at time t = 0,1,2, ..., n.

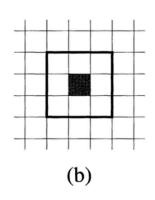
A rule  $R = \{R_1, R_2, ..., R_m\}$  that specifies the time evolution of the states  $\Phi(\vec{r}, t)$  in the following form:

$$\Phi_{j}(\vec{r}, t+1) = R_{j}\left(\Phi(\vec{r}, t), \Phi(\vec{r} + \vec{\delta}_{1}, t), \Phi(\vec{r} + \vec{\delta}_{2}, t), \dots, \Phi(\vec{r} + \vec{\delta}_{q}, t)\right)$$
(1)

where  $\vec{r} + \vec{\delta}_k$  denotes cells belonging to a specific neighborhood.

In the above definition, the rule *R* is applied to all sites simultaneously, leading to synchronous dynamics [34].

In the context of corrosion, the cell state can represent the presence of an element, a compound, or a corrosion product. The state of a cell changes over time depending on its own state and that of its nearest neighbors. Error! Reference source not found. shows a grid of cells where the cell undergoing a state change is represented in black, while the cells enclosed in a black frame (neighborhood) are the ones that influence this change, considering the state of their neighbors. This figure represents the three most used types of neighborhoods: Von Neumann, Moore, and Margolus. In the Von Neumann neighborhood (a), four neighbors are considered, located to the east, north, west, and south of the changing cell. On the other hand, in the Moore neighborhood (b), there are six neighbors surrounding the central cell. Finally, in the Margolus neighborhood, the change process is more complex as it depends on both space and time. Firstly, the space is divided into a 2x2 square. The first state change of cell *lr* occurs during an odd time, considering the neighbors in the upper square (*ul*, *ur*, *ll*, *lr*). In the next iteration, during even time, the state of cell *lr* is updated considering the neighbors in the square represented by dashed lines.



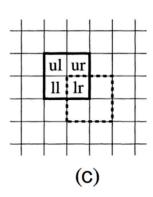


Figure 1. Most common neighboors. (a) Von Neumann. (b) Moore. (c) Margolus.

The neighborhood used traverses the entire grid, and through a set of transformation rules, the new state of each cell will be determined until the total update of the grid is completed, which represents the first generation (iteration) of the model. The rules and configuration of the AC model in corrosion simulations are specific for each phenomenon to be studied.

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## 2.1.1. Uniform Corrosion Model.

Fairén et al. [28] analyzed the evolution of surface roughness in the studied corroded metal. They examined the agreement between a classical macroscopic description and a mesoscopic approach that accounts for the development of such roughness. They studied how morphology could influence the modeling, finding that the model could simulate the mesoscopic heterogeneity of the electrode surface and its impact on the uniform corrosion process. Part of their study determined that further research was still needed to fully understand the relationship between the electrochemical mechanism involved, the steps determining corrosion rate, and the morphology of the electrode surface

Badiali et al. [35-37] studied the formation of films on a surface in the presence of corrosion, diffusion, and precipitation at the growth front. Obtaining results that show that the growth of the layer follows a parabolic law and that the model can be useful for predicting and controlling corrosion growth in metallic structures, pipes, and equipment, as well as for developing new corrosionresistant materials. Chen et al. [38,39] studied the corrosion and oxidation mechanism of stainless steel in lead-bismuth eutectic (LBE) environments, a liquid metal used as a coolant in some advanced nuclear reactors and accelerator-driven systems, and in [40] the medium was supercritical water. The model considered diffusion, reaction, and precipitation processes occurring on the steel surface, and a mesoscopic description was used to explore the general characteristics of the evolution of the involved processes. Additionally, they aimed to predict how oxide scale removal occurs and how it affects metal corrosion, concluding that the CA model is useful for understanding these mechanisms. Chen et al. [41] focused on simulating the growth of the oxide layer in chromium-containing stainless steels. Their objective was to verify whether the stochastic nature of the CA model for uniform corrosion would generate unstable or unreasonable results deviating from the deterministic model for uniform corrosion of steel in flowing LBE. Their results showed that the CA model is stable and reliable for simulating the thickness of the oxide layer. Chen et al [33] proposed a numerical simulation method to predict the evolution of uniform corrosion damage of the outer steel tube in concrete-filled tubular columns subjected to corrosive environments. They discussed the influence of solution concentration and the probability of dissolution of corrosive agents. The obtained results were compared with theoretical solutions and experimental findings. They concluded that different concentrations of corrosive agents have different impacts on the degree of corrosion damage. Ren et al. [42] simulated the uniform corrosion of aluminum in various environmental conditions. They defined corrosion rules based on the actual electrochemical reactions and examined the corrosion process at a mesoscopic scale. By studying the corrosion formation and modifying the rules for different concentrations of corrosive solutions and ambient temperatures, they gained insights into corrosion mechanisms. The simulation results contribute to a better understanding of corrosion and can aid in its prevention and mitigation, especially in aeronautical structures where corrosion can lead to fatigue-induced damage, compromising structural integrity. Li et al [43] sought to gain a better understanding of the corrosion evolution of marine structural steel in the tidal zone and how corrosion can be prevented or mitigated in this environment. Their objective was to comprehend the corrosion mechanisms in the tidal zone, identify the factors influencing the corrosion rate, and propose possible strategies to prevent or mitigate corrosion in structures and equipment used in marine environments, ultimately offering solutions to extend their lifespan. Wang et al [29,44] investigated the corrosion of a metal in molten chloride salt and explored methods to enhance its corrosion resistance. A simplified model was established based on the reactive diffusion of corrosive gas and the metallic substrate. Both experiments and simulations were conducted using the cellular automaton (CA) method.

The physical model from the experimental work determined that the main reactions involved are:

$$Cr + 2MgCl_2 + O_2 \rightarrow CrCl_4 + 2MgO \tag{2}$$

$$Ni + 1/2 O_2 \to NiO \tag{3}$$

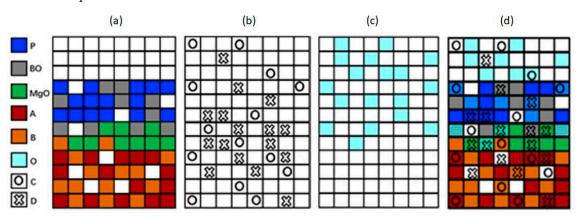
$$CrCl_4 + 2MgO + O_2 \rightarrow MgCr_2O_4 + Cl_2 + MgCl_2 \tag{4}$$

$$2Cl_2 + Cr \to CrCl_4 \tag{5}$$

They assumed the presence of corrosive substances in the molten salt from the beginning, where  $O_2$  and  $H_2O$  diffuse into the molten salt from the air, leading to the formation of HCl and  $Cl_2$  through a set of reactions. The dissolved  $O_2$  in the salt rapidly reacts with Cr (2). When the Cr content is insufficient,  $O_2$  reacts with Ni (3). The chloride containing Cr (mainly  $CrCl_4$ ) forms a protective spinel layer composed of  $MgCr_2O_4$  through (4). On the other hand,  $Cl_2$  can react with Cr, resulting in a chromium-depleted layer (5).

To establish the CA model, the chemical reactions involved in the corrosion process were simplified by assigning letters to the compounds or elements present. A = Cr; B = Ni;  $O = O_2$ ;  $C = Cl_2$ ;  $D = CrCl_4$ ; Mg = MgO;  $P = MgCr_2O_4$ ; BO = NiO.

The lattice sites were classified into fixed compounds (*A*, *B*, *MgO*, *P*, and *BO*) and mobile compounds (*O*, *C*, *D*). The interaction of mobile compounds within the lattice occurs through a probabilistic random walk process. As an example, Error! Reference source not found. shows four grid schematics of the CA model. In (a), a grid is depicted with the fixed compounds located. In (b), the location of mobile compounds that diffuse toward the metal is shown. In (c), the elements that can diffuse in the outer corrosion layer are present, and in (d), a lattice is shown where all compounds present in the process are located.



**Figure 2.** Schematics of the CA model. (a) Grid of fixed sites. (b) Grid of mobile sites that diffuse towards the metal. (c) Grid of sites that can diffuse in the outer corrosion layer. (d) General scheme of the grid in the CA model [29].

In reactions (6) to (9), the modified reaction and transformation rules for the CA model are shown.

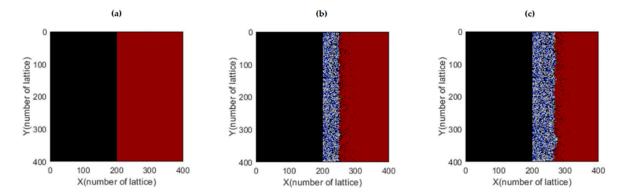
$$0 + A \rightarrow D + Mg0 \tag{6}$$

$$0 + B \to B0 \tag{7}$$

$$D + MgO + O \rightarrow P + C \tag{8}$$

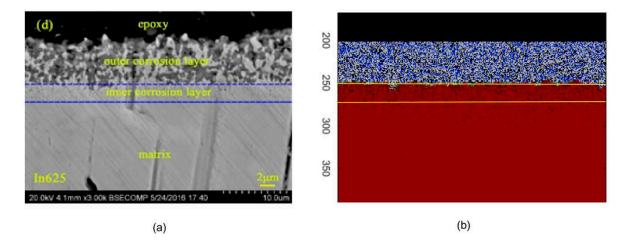
$$C + A \to D \tag{9}$$

The Margolus neighborhood was used to induce state changes in the different cells across generations. Error! Reference source not found. displays the results obtained by the model, where the left side (black color) represents the molten salt, while the right side (purple color) represents the metal under study. As the iterations progress, the growth of the oxide layer is observed. The number of iterations can be interpreted as representing an experimental time scale.



**Figure 3.** Simulation of corrosion layer growth at different iterations. (a) 40 iterations. (b) 25,000 iterations. (c) 36,000 iterations [29].

A comparison is shown in Error! Reference source not found. between the simulation results and a scanning electron microscopy (SEM) image. It was determined that 64,000 iterations correlate with the experimental results from 21 days of exposure, demonstrating that the AC simulation yields satisfactory results in the study of high-temperature corrosion of *Fe-Cr* alloys in the presence of molten salts.



# 2.1.2. Localized and pitting Corrosion model.

Localized corrosion encompasses corrosion processes that occur in specific areas of a material, leading to localized damage. Cellular automata simulate the initiation and propagation of localized corrosion, providing insights into factors influencing its occurrence, growth patterns, and evolution over time.

Di Caprio et al. [20,45] presented an electrochemical model for the corrosion of metals in contact with liquids, based on the description of chemical and electrochemical reactions occurring at the metal-liquid interface, which was simulated using CA. They investigated the corrosion process of each metallic site at the interface and compared the simulation results with experimental data. The proposed model reproduced experimental facts and trends without an explicit separation between anodic and cathodic sites. Overall, the study demonstrated that cellular automata-based models are a useful tool for simulating complex systems such as metal corrosion and can be adapted to include different rules and conditions according to the specific needs of the system under study. Cheng et al. [46] simulated the growth of metastable corrosion pits. The objective was to gain a better understanding of the mechanism behind the growth of these pits and compare the simulated results with experimental data. The researchers established a relationship between the current and current density of the pit over time to illustrate the mechanism of metastable pit growth. Additionally, they developed an optimal range of parameters for the simulation that allowed for visualizing the complete process of pit growth, including its geometry. The study built on previous work on the mechanism and electrochemical and mass transfer steps associated with the pitting corrosion process. Wang et al. [47] reproduced the interactions between metastable pits in stainless steel and analyzed how different factors affect their growth and stability. The model included corrosion, passivation, salt film hydrolysis, and hydrogen ion diffusion. Based on the model, they concluded that it is capable of accurately simulating the interactions between metastable corrosion pits in stainless steel. Wang et al. [48] investigated the interaction of metastable corrosion pits in stainless steel under mechanoelectrochemical effects using an updated cellular automaton/finite element model, elucidating the mechanisms for pit interactions. In the study, they considered an electrochemical system where stainless steel is exposed to an aggressive chloride solution. The stainless-steel samples had passive layers of surface oxide, which can be damaged in the presence of chloride anions. Two breakdown locations in the passive film were included to study only the pit propagation and not its nucleation. They concluded that the cellular automaton/finite element model used was effective in predicting the interaction of corrosion pits on a mesoscopic scale. Torska et al. [49] discussed the fracture dynamics in the investigated areas and performed a comparative analysis of pitting corrosion rates under real and simulated conditions. They demonstrated that the simulation procedure using cellular automata accurately reproduced the physics of corrosion. The study proposed a new modeling algorithm and local transition rules for the automaton cells used in simulating pitting corrosion images. Hu et al. [50] simulated pitting corrosion in nickel alloys. The authors employed four fundamental elements of the model to simulate electrochemical reactions, chemical reactions, and diffusion processes. The obtained results were qualitatively and quantitatively compared with experimental data and analogous findings cited in the literature. The study suggested that this type of model could be useful in gaining a better understanding of corrosion processes and developing corrosion-resistant materials for various industrial applications. Fatoba et al. [51] employed a combination of cellular automata and finite element analysis to simulate the growth of localized corrosion under the influence of applied stress. The results demonstrated that mechanical effects, such as plastic deformation, accelerated the rate of localized corrosion development. The study focused on low-alloy steel, but the findings may be applicable to other materials as well. Rujin et al. [52] established a mathematical model based on a statistical approach to describe the evolution process of pitting corrosion. Additionally, they proposed a 3D stochastic CA model to replicate the simultaneous initiation and

growth process of pits. The findings of the study can contribute to a better understanding of the laws governing pitting corrosion evolution and provide valuable insights into its prevention and control. To simulate localized corrosion, Pérez-Brokate et al. [31,53] aimed to gain a better understanding of hidden corrosion processes and pitting corrosion within corrosion cells by using a stochastic cellular automaton (CA) model. They studied the morphology, propagation, and influence of coupled diffusion within the corrosion cavity.

In the physical-chemical model, simplifications were made by assuming simplified electrochemical and chemical reactions (excluding contaminants and considering only  $H^+$  and  $OH^-$ ). Localized corrosion, being a multi-scale phenomenon, depends not only on atomic-scale surface phenomena but also on macroscopic environmental conditions.

The electrochemical reactions used:

Anodic reactions.

$$M + H_2O \rightarrow MOH_{aq} + H^+ + e^-$$
 (10)

$$M + OH^- \rightarrow MOH_{solid} + e^- \tag{11}$$

Cathodic reactions.

$$H^+ + e^- \to \frac{1}{2}H_2$$
 (12)

$$H_2O + e^- \rightarrow \frac{1}{2}H_2 + OH^-$$
 (13)

Authors called SJ reactions when the anodic and cathodic half reactions occur at the same location:

$$M + H_2O \rightarrow MOH_{aq} + \frac{1}{2}H_2 \tag{14}$$

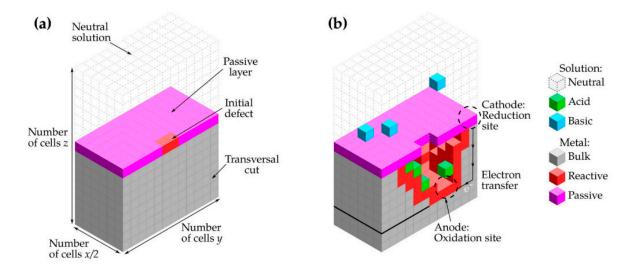
$$M + H_2O \rightarrow MOH_{solid} + \frac{1}{2}H_2 \tag{15}$$

$$MOH_{solid} \rightarrow MOH_{aa}$$
 (16)

The anodic and cathodic sites are electrically connected through the metal and the solution. When they are separated, they are referred to as Spatially Separated Electrochemical (SSE) reactions. The diffusion of SSE reactions results in the generation of  $H^+$  and  $OH^-$  ions, mimicking a random walk. When these ions interact, neutralization takes place, as depicted in the study through the following reaction:

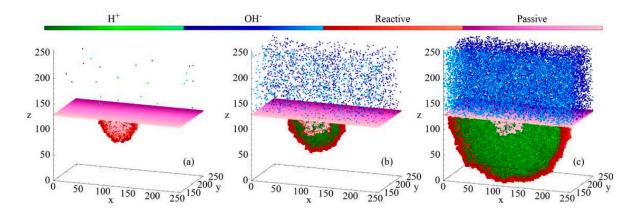
$$H^+ + 0H^- \to H_2 0$$
 (17)

The 3D lattice representation is depicted in Error! Reference source not found., illustrating a passivated metal in contact with a neutral electrolyte and the cathodic reaction takes place at a random point Figure 5a. The  $H^+$  and  $OH^-$  ions generated in the first reaction diffuse in the electrolyte. Each lattice site was determined by the dominant species. In Error! Reference source not found be the solid sites represent the metal (M), the metal in contact with the electrolyte (R), and the oxide layer providing passivity to the metal (P). Additionally, the electrolyte sites were differentiated into three different states based on pH. An acidic site (A), a basic site (B), and a neutral site (E) were considered. The Moore neighborhood was employed for the simulation.



**Figure 5.** Transversal view schema of (a) the initial global matrix and (b) after the development of the pit [30].

In Error! Reference source not found., they showed the evolution of the pit. They indicated the presence of an anodic half-reaction at the initial defect of the passive layer. The ions are dispersed randomly in the electrolyte, resulting in the growth of the pit when an H+ ion encounters the metal, leading to an electrochemical reaction. As the pit reaches a certain size, the concentration of acidic ions increases, causing instability and further enlargement of the pit.



**Figure 6.** Side views illustrating different pitting corrosion regimes (Ndiff = 2000): (a) initiation (for t  $\leq$  44,400), (b) growth instability phase (approximately 500 time steps, around t = 44,600), (c) stable growth (from t = 45,000) [30].

The model was considered a valuable tool for gaining a better understanding of localized and pitting corrosion processes and developing more effective strategies for corrosion prevention and treatment.

# 2.1.3. Stress Corrosion Cracking (SCC) model

Stress corrosion cracking is a phenomenon where the combination of tensile stress and a corrosive environment leads to crack initiation and propagation in a material. Cellular automata modeling the complex interactions between mechanical stress, electrochemical processes, and material degradation, helping to understand the conditions under which SCC occurs and its progression.

Zhu et al. [54] focused on predicting the service life of concrete bridges and preventing chloride-induced corrosion. They utilized 3D-CA, which accurately simulates chloride diffusion in concrete.

Multiple factors were considered, such as ambient relative humidity, temperature variations, stress, water-cement ratio (w/c), concrete degradation, corrosion propagation, cracks, and time. The study provides a useful tool for predicting the service life of the bridge and designing preventive measures against chloride-induced corrosion in concrete bridges. Liu et al. [55] modeled the SCC process in steel pipes. They employed a combination of finite element analysis and cellular automata techniques to simulate the initiation and propagation of cracks.

The electrochemical model used considered only the species  $H_2O$ , Fe,  $Fe^{2+}$ ,  $H^+$  and  $FeOH^+$ . The rules for corrosion evolution and cell diffusion were expressed in the following equations:

$$Fe \to Fe^{2+} + 2e^{-} \tag{18}$$

$$Fe^{2+} + 2H_2O \rightarrow FeOH^+ + 2H^+$$
 (19)

Based on the equations above, the authors formulated the rules of the AC model, where the diagram in Error! Reference source not found. represents the spatial layout of the model. The sites W represented a non-corrosive neutral solution ( $H_2O$ ), H represented a corrosive acidic solution ( $H^+$ ), the site M represented the metal, which dissolves to form site R after being in contact with the corrosive solution. The site R represents the active metal ( $Fe^{2+}$ ), and site P represents the corrosion product ( $FeOH^+$ ).

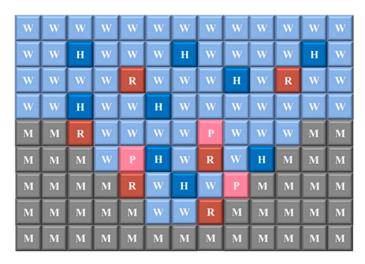
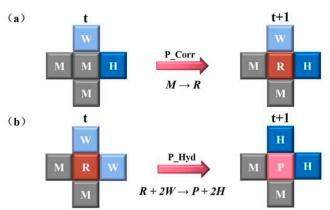


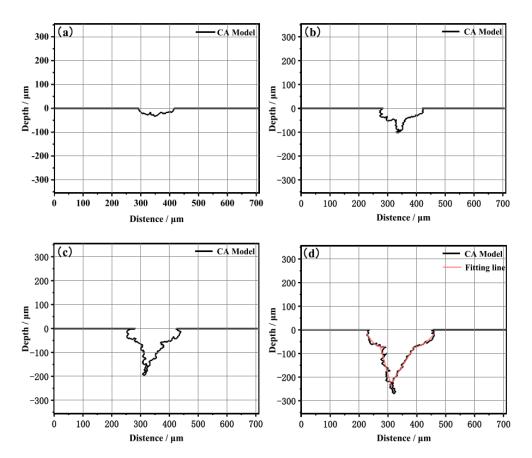
Figure 7. Schematic diagramo f the cellular automata spatial model [55].

The evolution rules for corrosion in the CA model were formulated based on the previous equations. Error! Reference source not found. shows the rules for the oxidation of Fe and the hydrolysis of  $Fe^{2+}$  to  $FeOH^+$ . When a site M is in contact with at least one site H, reaction 1 will occur with a corrosion probability  $P_{corr}$ , transitioning from site M to site R. Additionally, when a site R is in contact with at least two sites W,  $Fe^{2+}$  hydrolyzes to  $FeOH^+$  with a probability  $P_{Hyd}$ , and both site R and the two W sites are replaced by the corrosion site P and two H sites, respectively.



**Figure 8.** CA corrosion evolutions rules: (a) Oxidation of Fe to  $Fe^{2+}$  ions. (b) hydrolyzes  $Fe^{2+}$  ions to  $FeOH^+[55]$ .

The results demonstrated that prior to crack initiation, pitting corrosion was controlled by anodic reactions and mechanical factors, with electrochemical corrosion playing a significant role. During the crack propagation process, the mechano-chemical effects induced by plastic deformation promoted anodic dissolution at the crack tip, driving its propagation. This study may have significant implications for the pipe industry and help develop more effective strategies for corrosion prevention.



**Figure 9.** Evolution process of cross-sectional stress corrosion profiles: (a) 30 h, (b) 60 h, (c) 90 h, and (d) 120 h [55].

## 2.1.4. Intergranular Corrosion Model.

Intergranular corrosion occurs along the grain boundaries of a material, typically due to variations in composition or microstructure. Cellular automata can simulate the interactions between different grain boundaries, their susceptibility to corrosion, and the role of environmental factors in intergranular corrosion.

Chen et al. [56] developed a cellular automaton model to predict the susceptibility to intergranular corrosion in austenitic stainless steel and provide useful information on how to prevent or mitigate this problem. The results demonstrated how material properties change under different heat treatment and sensitization conditions. Additionally, they investigated factors affecting intergranular corrosion, such as the evolution of chromium-rich carbide precipitation and chromium concentration distribution [57]. They concluded that the CA model can be valuable for improving the design and performance of materials used in industrial applications.

Lishchuk et al. [58] utilized cellular automata to describe the propagation of intergranular corrosion and made simplifying assumptions that enabled them to predict the corrosion rate. The

results of the model demonstrated good qualitative and quantitative agreement with experimental data regarding the advancement of the corrosion front.

Jahns et al. [59,60] develop a simulation to predict internal corrosion during high-temperature applications in metal alloys. They utilized the model to describe diffusion-controlled precipitation processes and enhance the understanding of high-temperature corrosion in metal alloys. The researchers' goal was to develop more effective strategies to prevent or mitigate corrosion.

Di Caprio et al. [61–64] conducted various studies on intergranular corrosion using 2D and 3D CA models. Their aim was to predict the rate and pattern of corrosion in stainless steel exposed to corrosive solutions. They quantitatively analyzed the surface morphology of the steel and grain boundary structures. They presented CA methodologies to understand and prevent corrosion, and experimental validation yielded positive results.

Wang et al. [65] focused on investigating the corrosion behavior of a nickel-based alloy in a molten chloride salt mixture. The CA model enabled them to reproduce the distribution of corrosion products and components, as well as changes in the morphology and thickness of the corrosion layer over time. The results of the study can help predict the corrosion behavior of different metals in similar molten salt environments.

The mechanism of high-temperature corrosion is relatively complex. In the study conducted by Wang et al. [44], due to the alloy being primarily composed of *Cr*, *Fe*, and *Ni* elements, which play a significant role in corrosion resistance and alloy microstructure, only *Cr*, *Fe*, and *Ni* were considered in the model, excluding other elements present in lower concentrations.

The mechanism considered by the authors primarily involved the migration of metallic elements, substance consumption, and generation of corrosion products through the following equations:

$$Cr + O_2 \to Cr_2O_3 \tag{20}$$

$$Fe + O_2 \rightarrow Fe_2O_3 \tag{21}$$

$$Ni + O_2 \rightarrow NiO$$
 (22)

$$Cr + Cl_2 \rightarrow CrCl_4$$
 (23)

$$Fe + Cl_2 \rightarrow FeCl_3$$
 (24)

$$CrCl_4 + O_2 \rightarrow Cr_2O_3 + Cl_2 \tag{25}$$

$$FeCl_3 + O_2 \rightarrow Fe_2O_3 + Cl_2 \tag{26}$$

Like the presented studies in the uniform corrosion section, the physical model was simplified to facilitate the programming language.

$$EE + O \rightarrow YY \tag{27}$$

$$DD + O \to Y \tag{28}$$

$$AA + O \rightarrow AO \tag{29}$$

$$EE + c \to D \tag{30}$$

$$DD + c \to FF \tag{31}$$

$$D + O \rightarrow YY + c \tag{32}$$

$$FF + O \rightarrow Y + c \tag{33}$$

where: AA = Ni, DD = Fe, EE = Cr, O = O2, c = Cl2, Y = Fe2O3, YY = Cr2O3, AO = NiO, D = CrCl4, and FF = FeCl3. All elements except for O, c, and D were considered fixed in the lattice. The positions of O and C were randomly predetermined with an assigned probability, and the sites AA, DD, and EE represent the alloy elements.

To consider the simulation of intergranular corrosion, the authors evaluated the effect of grain size. To obtain the initial structure, they simulated the grain growth process at different time steps Error! Reference source not found..

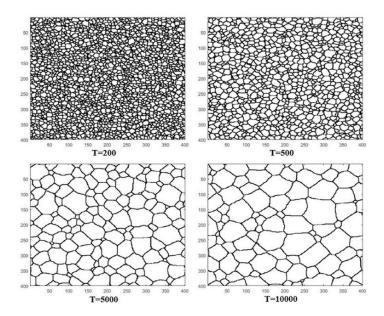
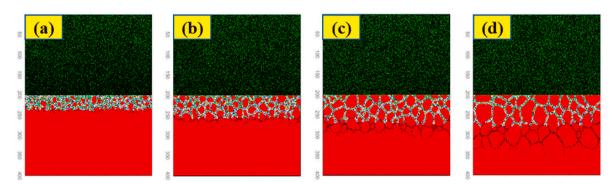


Figure 10. Grain growth process at different simulation time steps [44].

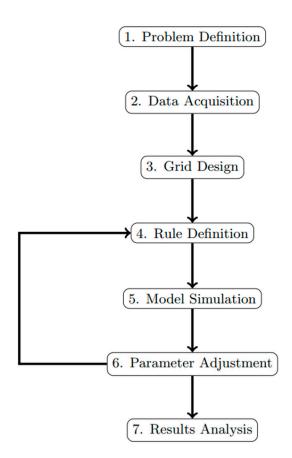
Therefore, their simulation of intergranular corrosion consisted of obtaining the initial microstructure model, which was combined with the AC model. The result of the model is shown in Error! Reference source not found., which displays different structures of the model at various iterations. The development of intergranular corrosion in the studied steel by the researchers can be observed.



**Figure 11.** The simulation results of intergranular corrosion (T = 70000) of the initial structure obtained at different simulation time steps:(a) T = 500 (b) T = 1000 (c) T = 2000 (d) T = 5000 [44].

# 3. Modeling approach and methodology for simulating corrosion phenomena

The methodology for simulating corrosion phenomena involves several key steps and considerations.



- Identify relevant corrosion aspects and interactions with materials, propagation, and environmental factors.
- Collect data on material properties, environmental conditions, and electrochemical parameters.
- 3. Determine grid type (2D or 3D) and assign states to cells based on the problem.
- Define rules for cell interaction and state changes based on neighbors.
- Implement cellular automaton using programming language with defined rules and grid.
- Conduct model experiments, explore configurations, and adjust parameters.
- Analyze results, compare with observations, validate the simulation, and consider model improvements.

Figure 12. Methodology for implementing a cellular cutomata model.

**Table 1.** Summary of the results published.

CA	Neighborho	Model	Boundar	Lattice	Rul	Cycles	Corrosion	Environme	Materi	Temperatur	Exposure	Validation	Ref.
type	od	type	y	size	es	Cycles	type	nt	al	e (°C)	time (h)	type	
LGAª	n-vector	Probabili stic	Periodic	-	-	-	-	-	-	-	-	Boltzmann hypothesis	[66]
2D	n-vector	Probabili stic	Periodic	200x160	3	48.000	Kinetic of internal oxide precipitati on	Oxygen	Metal	-	-	Theory of phase equilibriu m	[67]
Theoret ical	Moore	Probabili stic	Periodic	> 1000x1000	8	-	Uniform	Electrolyte	Metal	-	-	Previous work data	[28]
2D	Von Neumann	Probabili stic	Periodic	2000x1000	2	10.000 to 90.000	Uniform	Electrolyte	Metal	-	-	-	[35]
2D	Von Neumann	Probabili stic	Periodic	1000×1000	3	200.000	Uniform	Solvent	Metal	-	-	Parabolic law	[36]
2D	Von Neumann	Determi nistic	Periodic	600x20000	2	150	Uniform	Electrolyte	Metal	-	-	Mott and Cabrera Parabolic's law	[37]
2D	Von Neumann	Probabili stic	Periodic	1000x1000	2	25.000	Uniform	Liquid lead alloy	Metal	550	3.000	Wagner theory	[38]
3D	-	-	-	100×100	-	-	Intergranu lar	Sulfuric acid	Metal	1100	0-400	Electroche mical potentiody namic reactivatio	[56]
2D	Moore	Probabili stic	-	500x500	2	200.000	Uniform	LBE	Metal	535	3000	Wargner theory	[39]
LGA- 2D	Von Neumann	Probabili stic	-	2000xLy	3	-	Pasivation	Solution	Metal	-	-	Passivatio n theory	[68]

2D	Moore	Determi nistic	-	200x200	2	3	Intergranu lar	Solution	Metal	1100	2	-	[57]
2D	Von Neumann	Probabili stic	Periodic	-	2	7.200.000	Localised	Solution	Metal	360	-	Experimen tal	[45]
2D	Von Neumann	Probabili stic	-	1000×1000		399.577	Localised	Solution	Metal	-	-	Pistorius experimen tal results	[46]
2D-3D	Moore	Probabili stic	Periodic	640x320 - 240x280x2 40	3	-	Intergranu lar	Solution	Metal	-	144	Eperiment al	[58]
LGA- 2D	Von Neumann	Probabili stic	-	2000xLy	2	-	Pasivation	Solution	Metal	-	-	Passivatio n theory	[69]
2D	Moore	Probabili stic	-	500x500	2	5.000	Uniform	Water	Metal	600	1000	Experimen tal	[40]
2D	Von Neumann	Probabili stic	Periodic	900x300	2	70.000	Uniform, localised	Solution	Metal	300-360	-	Experimen tal	[20]
2D	Von Neumann and Moore	Probabili stic	Periodic	1000×1000	14	7.679	Localised, passivatio n	Solution	Metal	-	-	Theoretica l corrosion and passivity phenomen a	[70]
2D	Von Neumann and Moore	Probabili stic	Periodic	1000x1000	11	4.000	Crevice, passivatio n	Solution	Metal	-	-	Experimen tal	[71]
2D	Moore	Probabili stic	-	500x500	2	200.000	Uniform	LBE	Metal	-	-	Chi-square of goodness- of-fit	[41]
2D	Von Neumann and Moore	Probabili stic	-	512x512	3	2.000	Oxidation and nit	-	Metal	1100	100	Experimen tal data	[72]

3D	Moore	Probabili stic	Periodic	151x200x2 00	3	200	Pitting	Solution	Metal	-	0.5	Experimen tal data	[73]
2D	Von Neumann and Moore	Probabili stic	-	512x512	3	20.000	Oxidation and nitridation	Solution	Metal	1100	100	Experimen tal data	[74]
3D	Moore	Probabili stic	Periodic	-	4	124	Pitting	Solution	Metal	-	480	Experiman tal data	[75]
2D	Moore and Von Neumann 2nd order	Probabili stic	-	1000x1000	4	1.000	Pitting	Solution	Metal	-	-	Experimen tal data	[76]
2D	Von Neumann	Probabili stic	-	1024x1024	2	-	Pitting	Solution	Metal	-	-	Experimen tal data	[47]
2D	Moore	Determi nistic	Reflect	-	2	-	Pitting	Solution	Metal	-	-	Experimen tal data	[77]
2D	Von Neumann	Probabili stic	Periodic	1024x1024	5	-	Pitting	Solution	Metal	-	-	Experimen tal data	[48]
2D	Von Neumann 2nd order	Probabili stic	-	-	3	-	Pitting	Solution	Metal	Room	-	Experimen tal data	[49]
2D	Von Neumann	Probabili stic	Periodic	2000x2000	3	6.000	Pitting	Water	Metal	-	1.600	Experimen tal data	[50]
2D	Von Neumann and Moore	Probabili stic	-	500x500	3	3.000	Intergranu lar	Air	Metal	1100	100	Experimen tal data	[59]
3D	Moore	Probabili stic	-	512x512x5 12	4	> 5.000	Occluded, localized	Solution	Metal	-	-	Experimen tal data	[53]
3D	-	Probabili stic	Periodic	512x512x4 096	-	4.000	Intragranu lar	Solution	Metal	-	7.000	Experimen tal data	[61]
2D	Von Neumann	Probabili stic	-	-	3	25.000	Electroche mical oxidation	Solution	Metal	600	30	Experimen tal data	[78]

2D	Von Neumann and Moore	Probabili stic	-	512x512	3	-	Intergranu lar oxidation	Air	Metal	1100	100	Experimen tal data	[60]
2D	Moore and Von Neumann extend	Probabili stico	Periodic	1000x1000	-	2.000	Uniform	Solution	Metal	-	-	Theoretica l and experimen tal	[33]
3D	Moore	Probabili stic	-	256x256x2 56	7	45.000	Pitting	Solution	Metal	-	-	Experimen tal data	[31]
3D	Moore	Probabili stic	Periodic	512x512x5 12	7	7.000	Generalize d	Solution	Metal	-	-	Experimen tal data	[79]
CA-FE- 2D	Moore	Probabili stic	-	2000x1000	4	-	Localized	Solution	Metal	-	-	Experimen tal data	[80]
3D	Von Neumann	Probabili stic	Constant and periodic	100x100x1 00	4	400	Atmosphe ric corrosion	Atmosphere	Metal	-	-	Theoretica l and experimen tal data	[81]
3D	Von Neumann	Determi nistic	Periodic	100x100x1 00	5	1.000	Uniform	Solution	Metal	20	-	-	[42]
3D	Von Neumann	Probabili stic	-	7500x7500 x1500	-	-	Pitting	Salt-Spray	Metal	35	1.440	Experimen tal data	[52]
2D	Margolus	Probabili stic	Rigid	400x400	4	25.000	Uniform	Solution	Metal	600	504	Experimen tal data	[29]
LGA- 3D	Von Neumann	Probabili stic	Periodic	-	-	-	Passivatio n	Solution	Metal	-	-	Passivatio n theory	[82]
3D	12- neighbors	Probabili stic	Periodic	1280x1280 x1280	-	-	Intergranu lar	Solution	Metal	-	2.000	Experimen tal data	[62]
2D-bi plane	Von Neumann	Probabili stic	-	500x500	5	100	Pitting	Solution	Metal	-	-	Experimen tal data	[83]
3D	-	-	-	2048x2048 x256	3	350	Intergranu lar	Solution	Metal	-	-	Experimen tal data	[63]

2D	Margolus	Probabili stic	Periodic	400x400	7	70.000	Uniform, intergranu lar	Solution	Metal	600	504	Experimen tal data	[44]
3D	Margolus	Probabili stic	Periodic	1280x1280 x1280	-	21.555	Intergranu lar	Solution	Metal	111	17.783	Experimen tal data	[64]
2D-3D	Margolus	Probabili stic	Periodic	40x400 - 100x100x1 00	10	50.000	Intergranu lar, pitting	Solution	Metal	700	168	Experimen tal data	[65]
3D	Von Neumann	Probabili stic	Periodic	1000x1000 x1000	5	-	Uniform, pitting	Solution	Metal		168	Experimen tal data	[43]
2D	Moore	Probabili stic	-	1024x1024 x128	4	2.000.000	Aqueous	Solution	Metal	50	853	Experimen tal data	[84]
2D	Von Neumann	Probabili stic	-	250x250	2	2.000	Cracking	Solution	Metal	27	-	Experimen tal data	[55]
3D	Von Neumann	Probabili stic	-	2000x2000 x1000	2	-	Cracking	Concrete	Metal	23	672	Experimen tal data	[54]
3D	Moore	Probabili stic	Periodic	104x104x1 04	5	-	Atmosphe ric corrosion	Atmosphere	Metal	-	-	Experimen tal data	[30]

# 4. Future Perspectives and Emerging Trends.

Cellular automata models have emerged as powerful tools for analyzing various types of corrosion, offering valuable insights into their complex behavior. These models capture spatial and temporal variations, enabling a thorough examination of corrosion phenomena. Notably, cellular automata models have successfully analyzed specific corrosion types such as stress corrosion cracking, corrosion under insulation, marine corrosion, and more. Through these simulations, critical areas prone to corrosion can be identified, corrosion control measures can be evaluated, and corrosion-induced failures can be predicted, providing valuable perspectives for effective corrosion management.

When developing cellular automata models to simulate corrosion phenomena, it is crucial to consider a range of environmental parameters that have a substantial impact on corrosion performance. These parameters reflect the realistic conditions under which corrosion takes place. Firstly, the composition of the electrolyte solution surrounding the material holds the utmost importance in determining the corrosive environment. Factors such as pH, chloride concentration, dissolved oxygen levels, temperature, and other relevant chemical species all contribute to this environment. Secondly, the movement of the electrolyte solution, also known as flow or mass transport, plays a significant role in corrosion processes. It is imperative to account for these parameters in order to create accurate and comprehensive cellular automata models for studying corrosion behavior. Consideration of flow patterns, velocity, and diffusion rates within cellular automata models is essential to simulate the effects of convection, mass transfer, and concentration gradients on corrosion behavior. Thirdly, these models should account for the specific environmental exposure conditions relevant to the corrosion scenario, such as marine environments, industrial atmospheres, underground conditions, or exposure to specific chemicals. The inclusion of temperature as a critical environmental parameter is crucial, as thermal effects can impact corrosion rates by influencing electrochemical reaction kinetics, diffusion rates, and material properties. By incorporating temperature variations into the cellular automata model, a more comprehensive understanding of corrosion behavior under different thermal conditions can be achieved.

In some corrosion scenarios, such as atmospheric corrosion, humidity, and moisture levels play significant roles. A well-designed cellular automata model enables the simulation of localized corrosion phenomena related to moisture accumulation or the presence of electrolyte films. Additionally, it is important to consider the influence of ultraviolet (UV) radiation from sunlight, especially in outdoor environments. UV radiation can induce photochemical reactions, affect surface properties, and alter the electrochemical behavior of materials. Therefore, incorporating the effects of UV radiation into the cellular automata model provides a more accurate representation of corrosion behavior. By considering these various environmental parameters and incorporating them into the cellular automata models, a comprehensive and realistic simulation of corrosion behavior can be achieved, facilitating a deeper understanding of the corrosion processes and aiding in the development of effective corrosion mitigation strategies. Through the evaluation of corrosion mechanisms, the development of corrosion prevention strategies, and the assessment of material performance in specific environments by cellular automata models, researchers can obtain a more comprehensive understanding of corrosion processes and accurately simulate the behavior of materials under realistic conditions. The integration of data-driven approaches, such as machine learning and artificial intelligence, enhances corrosion monitoring, prediction, and decision-making are fundamental for a good future in the early detection of failures. These approaches leverage large datasets to identify patterns, anomalies, and correlations that can improve corrosion management strategies. Advances in remote sensing technologies and real-time monitoring systems enable continuous and remote monitoring of corrosion parameters and provide valuable data for proactive corrosion management, allowing for early detection of corrosion, timely interventions, and improved asset integrity management.

The future of cellular automata in corrosion research will be about the integration of advanced computational techniques, such as machine-learning algorithms, and data-driven approaches. This integration allows for more accurate and predictive corrosion models by leveraging large datasets

and optimizing model parameters based on experimental or real-time monitoring data. In addition, the incorporation of electrochemical considerations in cellular automata models can better capture the fundamental mechanisms and behavior of corrosion, leading to more realistic simulations and predictions. The multi-scale modeling is a growing trend toward coupling cellular automata models with other modeling techniques, such as finite element analysis or computational fluid dynamics.

The integration of cellular automata in corrosion management generates models with corrosion monitoring and control systems that will enable real-time feedback and adaptive control strategies. This integration can enhance the effectiveness of corrosion prevention and mitigation measures by dynamically adjusting parameters based on the evolving corrosion behavior. Real-time monitoring techniques in cellular automata models allow for dynamic modeling of corrosion processes. By integrating data from sensors and monitoring systems, researchers can obtain more accurate and upto-date information on corrosion behavior, enabling proactive corrosion management strategies. At the same time, the focus is on refining model parameters, algorithms, and simulation techniques to improve the accuracy and reliability of predictions, ultimately enabling more effective corrosion management strategies. CA models have the potential to be used in the design and optimization of corrosion-resistant materials used in storage energy by molten salts. Future perspectives in cellular automata models in molten salt corrosion involve the development of more sophisticated models that can accurately capture the complex corrosion mechanisms specific to molten salt environments. This includes considering factors such as electrochemical reactions, mass transport, and the interaction between molten salts and the material surface.

## 5. Conclusions

In conclusion, cellular automata offer a promising avenue for advancing corrosion management through their provision of a robust modeling and simulation framework. Their capacity to effectively capture the intricate dynamics of corrosion processes presents an opportunity to develop predictive models, corrosion-resistant materials, and real-time monitoring systems. Although challenges remain to be addressed, the prospects of utilizing cellular automata in corrosion management appear encouraging. Continued research and development in this field hold the potential for significant advancements in corrosion control and prevention.

- Most studies focus on uniform corrosion, localized corrosion, and intergranular corrosion. These
  three mechanisms account for almost 80% of all studies to date, leaving other types of corrosion,
  such as stress cracking corrosion, with only around 4% of the found studies. This indicates that
  there is a gap to be explored using cellular automaton for other existing corrosion mechanisms.
- On the other hand, it is observed that the CA model in all reviewed studies has a similar structure. It starts with a known phenomenon, either theoretical or experimental, which is sought to be simulated using CA. Then, the physicochemical or electrochemical model that governs the process is defined, and it is translated into a simplified language that facilitates programming. Each study generates its own reaction and transformation rules, dependent on the initially proposed physicochemical or electrochemical model so that these rules can simulate the desired process.
- There is variability in the mesh size used, the boundary conditions, the type of neighborhood utilized, or the number of transformation rules. Each study considers these aspects in a personalized manner, seeking the suitability of the result depending on the complexity of the corrosion process being studied. Therefore, there is still no single rule that encompasses all processes in a single comprehensive CA model.
- Most studies conclude that the CA model has tremendous potential for simulating the corrosion
  process of different alloys under different conditions. By using simple rules, it can generate
  complex patterns, and the obtained results closely match the experimental behavior.
  Furthermore, the model's ability to represent multiple types of physical phenomena makes it a
  powerful tool that can help researchers see the studied phenomena from a different perspective.

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