

SIMULATION OF DIFFUSION PROCESSES IN LABYRINTHIC DOMAINS BY USING CELLULAR AUTOMATA

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ABSTRACT

Components of gas turbines are exposed to different damaging factors during their lifetime. Besides the mechanical stress caused by the high centrifugal force another important attack is initiated by the surrounding gas atmosphere. At high temperatures gas molecules dissociate and the atoms diffuse inwards the metallic components and react with the solved alloy constituents. The reaction products precipitate inside the component and pose an obstacle for the succeeding gas atoms. In order to analyse this effect this process has been projected onto a cellular automaton. For that purpose an existing diffusion model has been selected and an extension to handle obstacles has been developed. This extension has been inspected thoroughly and its sensitivities regarding its parameters have been explored.

INTRODUCTION

High temperature corrosion (HTC) is a damage process which occurs where metallic materials get into contact with gas atmospheres at high temperatures, e.g. gas turbines in power plants (Krupp 1999). This process can be divided into external and internal corrosion where the internal process is the critical one, since it can only be observed with difficulties.

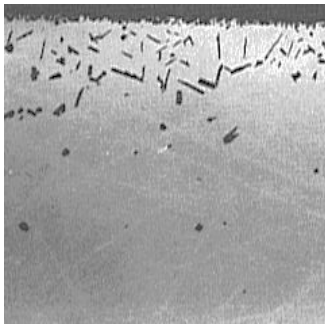


Figure 1: Cross-section of a nickel-base alloy with nitride precipitations

HTC can be regarded as an interaction of two elementary processes, inwards oriented diffusion of dissociated gas atoms on the one hand and the chemical reaction between these gas atoms and the alloy components on the other hand. The reaction products are oxides and nitrides that remain at the location inside the material where they precipitate. Figure 1 shows a cross-section of a specimen which evinces internal precipitations. These oxides and nitrides cause changes of the microstructure and this in turn can lead to failure of the attacked structure element.

The kinetics of this corrosion process is mainly determined by the gas diffusion towards the reaction zone. Since the high temperatures provide lots of thermal energy the chemical reaction accelerates and so the reaction takes place almost instantaneously. Thus the amount of available gas atoms is the primal factor that limitates the process. When the formation of internal precipitation has consumed all existing alloy ingredients until they are locally exhausted, the precipitation front moves on inwards. As a consequence the gas atoms have to diffuse a larger distance from the surface to reach the reaction zone and their courses are more and more bulked by precipitations.

From the macroscopic point of view this effect leads to a change of the diffusion velocity (Schnaas 1978). The aim of this work is to examine the diffusion in the region of the precipitations and to give an evidence for the influence of the oxides and nitrides on the gas diffusion. It is intended to express this influence as an effective diffusion coefficient inside the precipitation zone. The heterogenous occurrence of oxides and nitrides will be represented by a homogenized coefficient. By using this coefficient in a homogenized domain the influence of the microscopic obstacles could be regarded in a macroscopic way. With that it is possible to transfer various geometries, locations and orientations of the precipitations into one system depended quantity.

DIFFUSION MODEL

Diffusion is a kinetic process which reduces the concentration gradient of chemical components inside a phase.

Contrary to the diffusion in liquid media, where the diffusion is not restricted, the diffusion in solids, particularly with regard to metals, is adapted to the atomistic structure. Regarding the diffusion microscopically there are some elementary mechanisms that govern the transport in atomistic scale. The most important mechanisms are interstitial, ring and vacancy-assisted diffusion. From the macroscopic point of view the mass flux can be expressed as a vector field \mathbf{j} as noted in Equation (1). Its magnitude is proportional to that mass quantum which flows during a unit time through a unit area. The constant coefficient D describes the extent of the flux caused by the concentration gradient:

$$\mathbf{j} = D \nabla c \quad (1)$$

Regarding the mass conservation in a finite volume element and assuming that in the domain there is neither a mass sink nor a source, the divergence of the mass flux is the only term which changes the concentration inside the volume, as expressed in Equation (2):

$$\frac{\partial c}{\partial t} = -\nabla \cdot \mathbf{j} \quad (2)$$

Combining the mass conservation and the mass flux leads to Fick's 2nd law (3), relating the temporal variance of the concentration to the second spatial derivation of the concentration profile. In cases of isotropic diffusion the factor D can be reduced to a scalar coefficient, otherwise it becomes a diffusion tensor.

$$\frac{\partial c}{\partial t} = D \Delta c \quad (3)$$

Since Fick's 2nd law is a partial differential equation with only a few analytical solutions available for special cases, numerical methods have to be used to apply it to technical problems. Nevertheless one significant analytical solution needs to be presented here (Glicksman 2000). Regarded is a 1-dimensional half space. At the left boundary the constant concentration is c_Γ and the initial concentration on the domain is assumed to be zero. For these conditions an analytical solution of Fick's 2nd law is given by Equation (4):

$$c(t, x) = c_\Gamma \cdot \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \quad (4)$$

This time- and position-dependent solution will be used to validate the implementation of the cellular automaton and to evaluate the results of the simulations.

EXPERIMENTAL PROCEEDING

To describe the diffusion in the range of the precipitations in a macroscopic way an effective diffusion coef-

ficient has to be developed. It has to represent the diffusion conditions inside the region of obstacles. The diffusion across this range will be modelled by means of cellular automata. Performing simulations with this method will result in concentration profiles across the precipitation zone as well as the undisturbed area behind it. By fitting the parameter D of the analytical solution in Equation (4) with the concentration profile in region of obstacles an effective diffusion coefficient D_{eff} can be determined. Relating this coefficient to the coefficient D of the undisturbed region leads to the labyrinth factor Γ as introduced in Equation (5).

$$\Gamma = \frac{D_{\text{eff}}}{D} \quad (5)$$

This quantity expresses the extent of obstruction caused by the precipitations. Since it is impossible to get universal results for all possible geometries of obstacles with this method the simulations will be performed with selected test configurations. However, these results can be interpreted as indicators concerning the diffusion behaviour in technically relevant systems.

CELLULAR AUTOMATA

Cellular automata are mathematical models which describe the dynamics of spatially distributed systems with simple rules on given domains (Gaylord 1996). Hence, they can be alternatively applied in those disciplines where up to now only partial differential equations have been used in combination with FEM. However the cellular automata are more advantageous concerning to complex geometrical structures and the possibility of handling obstacles and several phases only by changing the policies.

A sophisticated approach to simulate diffusion process with means of cellular automata was introduced in (Chopard and Droz 1998). In this model the cells can be occupied by a maximum of 4 particles provided that the regarded domain is 2-dimensional. In a 3-dimensional domain this number increases to 6 corresponding to the number of closest neighbour-cells. The discrete values specify the number of particles inside a cell. A fundamental problem of this approach is to guarantee that the number of particles inside a cell is not more than the admitted one. To elude these difficulties the iterating evaluation is divided into the two phases mixing and moving.

In the first phase the incoming particle vectors are processed. From this starting configuration the sequence of outwards oriented particle vectors can be determined for each cell as permutations of those which came in. In 2 spatial dimensions $(2 \cdot 2)! = 24$ permutations are possible in principle. However this approach is restricted to 4 configurations as shown in Figure 2.

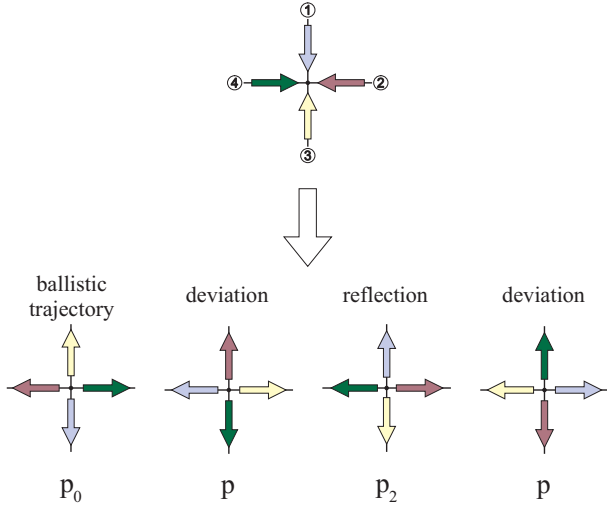


Figure 2: Possibilities of particle movement in the model of Chopard and Droz

The probability of these potential permutations can be weighted separately. It is postulated that the probability of a 90° deviation is independent of the rolling direction and so the two parameters for both possibilities can be combined together to only one called p . In addition the probability of a ballistic trajectory is denoted as p_0 and for reflection with p_2 . Summing up all probabilities must result in 1. Another constraint is that none of the probabilities is allowed to be zero.

$$p_0 + 2p + p_2 = 1, \quad p, p_0, p_2 > 0 \quad (6)$$

With these parameters it is possible to influence the behaviour of the cellular automaton considerably. Increasing p_0 and consequently decreasing p and p_1 leads to a high velocity of the diffusing particles. Chopard succeeded to show that the cellular automaton indeed converges to a Fick diffusion process when both the spatial increment Δx and the time step Δt tend to zero. Moreover he derived a functional correlation between the set of probabilities and the diffusion coefficient as shown in Equation (7):

$$D = \lim_{\Delta t \rightarrow 0, \Delta x^2 \rightarrow 0} \left(\frac{\Delta x^2}{\Delta t} \cdot \frac{p + p_0}{4(1 - p - p_0)} \right) \quad (7)$$

With validity of Equation (6) in mind, the probabilities p , p_0 and p_1 can be varied. By this means the diffusion coefficient of the particles can be adjusted without changing the grid and time step.

VERIFICATION OF THE IMPLEMENTED CELLULAR AUTOMATA

For this approach the comparison between the cellular automaton results and the analytical solution (4) of the diffusion equations has been carried out. For this pur-

pose a 2-dimensional cellular automaton has been implemented in MATLAB. With this the configurations as discussed for the analytical solution (4) have been imitated and simulations have been performed with 100 repetitions. To make a comparison between the 2-dimensional results with the 1-dimensional analytical solution possible, the average concentrations depending to the distance from surface have been evaluated. In Figure 3 the different states of the cellular automaton and the according analytical solutions are shown.

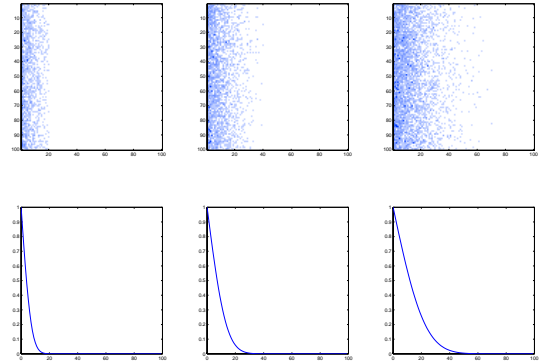


Figure 3: Comparison between the analytical solution and the output of the cellular automaton

To analyse the results statistically the concentration profile of the last time step is regarded again. In addition to this the 98% confidence interval has been exemplary computed and plotted in Figure 4 for this simulation series. It shows the narrow confidence range that widens a bit far from surface. This can be led back to the numerical inaccuracy.

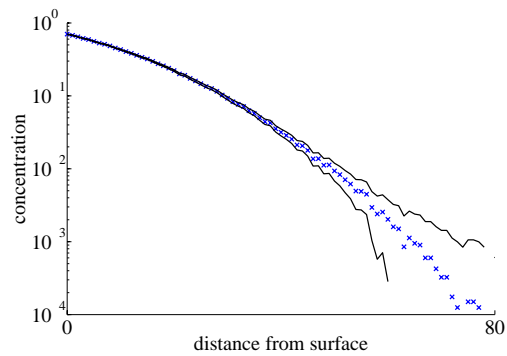


Figure 4: CA- results with its 98% confidence range

EXTENSION TO DOMAINS WITH OBSTACLES

Since the basic model of Chopard and Droz does not consider the treatment of obstacles, new rules to handle those disturbances of diffusion were added. It is important that the rules of the cellular automata were only supplemented with this new aspect, but not changed. So the proven physical correctness in the free volume is maintained. In the presence of one adjacent obstacle four cases have to be discerned as shown in Figure 5.

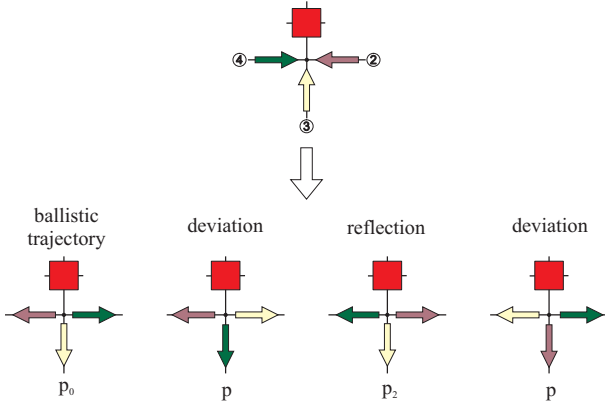


Figure 5: CA policy concerning one adjoining obstacle

To follow the exclusion principle only three particles are admissible in the regarded cell. Analogous to the basic model the output directions are determined by the permutations of the particle vectors in conformity with their probabilities. If two obstacles are adjoining to a cell the only two different possible configurations are illustrated in Figure 6.

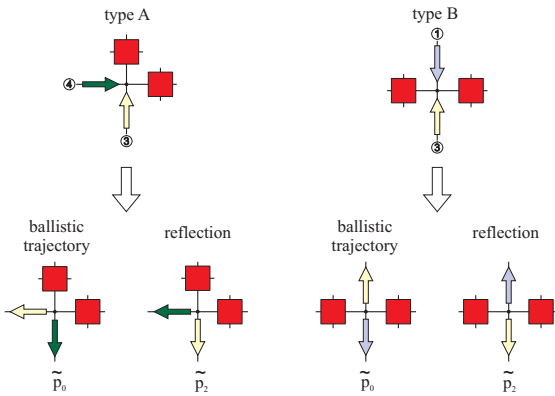


Figure 6: CA policies concerning two adjoining obstacles

In the first scene constituted as type A two obstacles are close to each other. Even though a straight-line course is impossible in this case, the only potential permutation is still called ballistic trajectory. The other arrangement of two obstacles is an opposition denoted as type B. Here it is clear, that no deviation can take place. As a consequence the probabilities for the admitted particle vectors have to be recalculated as realized in Equation (8):

$$\tilde{p}_0 = \frac{p_0}{p_0 + p_2}, \quad \tilde{p}_2 = \frac{p_2}{p_0 + p_2} \quad (8)$$

The last two remaining configurations are quite straightforward. If three obstacles are neighbouring a cell, the only possible particle vector will be inverted. And finally in the case of four obstacles no particle can get into the cell.

PARAMETER VARIATIONS

The aim of the following investigations is to ascertain the influence of the numerical and physical parameters on the simulated diffusing behaviour. For this purpose a special 2-dimensional test arrangement has been designed. At the initial state only blocks of obstacles are arranged in the examined domain. They are assumed to be immobile. The boundary conditions for the bottom and the top are supposed to be cyclic. The right boundary is determined to be isolated and at the left hand side a constant density of particles is defined. This can be effected by deleting the actual content of the cells in the first column and assigning them by a random generator adjusted with the required probability at the beginning of each iteration. Figure 7 shows the final state of the cellular automaton.

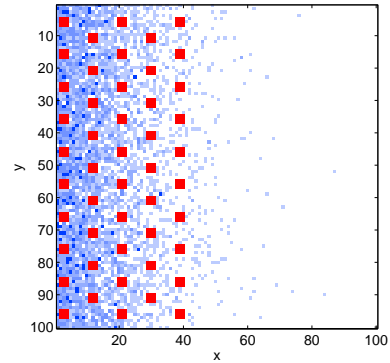


Figure 7: Diffusion CA with obstacles

In the range of the obstacles the diffusion is hampered. To quantify this effect an effective diffusion coefficient for this range has to be determined as explained below.

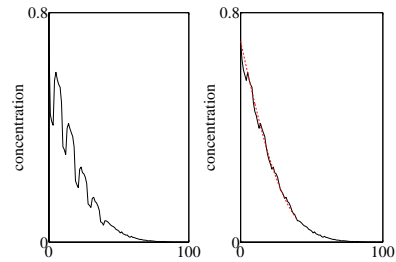


Figure 8: Evaluation of raw CA results. 8a (left): Without correction. 8b (right): Corrected for reduced volume due to obstacles

Firstly the raw concentration profiles as shown in Figure 8a have to be corrected. In the first evaluation step the obvious defect caused by reduced volume due to the obstacles has to be corrected. This can be adjusted by relating the average concentrations to the actual area the particles have at their disposal for diffusion. With these corrected values the parameter D_{eff} can be calculated with means of the least square method in the range of obstacles as shown in Figure 8b. With this quantity a

labyrinth factor Γ can be calculated as shown in Equation (5). It relates the measured effective diffusion coefficient with the adjusted one.

SIMULATION EXPERIMENTS

Regarding Equation (7) again it is apparent, that there are in principle two different ways to determine the diffusion coefficient D . At first the ratio of the time step width Δt and the spatial increment Δx can be varied. Increasing Δx leads to an increasing diffusion coefficient and analogue decreasing Δt . Since the implemented cellular automaton consists of a fixed grid the variation of this quotient will be performed by changing the time step size. The second way to adjust the diffusion coefficient is to change the relation between the probabilities p , p_0 and p_2 when the range of settings is restricted by Equation (6).

In order to analyse the consequences of adjusting in both ways several simulations have been carried out. In a first test series the diffusion coefficient has been determined with three different time step sizes. To get comparable results the number of time steps n_t for a given simulation duration have to be adapted. In the second test series the same diffusion coefficients as above have been adjusted by means of varying the set of probabilities. In Table 1 the results of the performed simulations are shown.

Table 1: Varying diffusion coefficients with the time step size and set of probabilities

D	200	400	600
n_t	800	1600	2400
Γ	0.81	0.79	0.77
p_0	0.1	0.4	0.6
Γ	0.96	0.83	0.70

Comparing the results a tendency is obvious in both tests. An increasing diffusion coefficient effects a decreasing Γ . Considering the ratio in Equation (5) this means, that the extent of obstruction increases with a increasing velocity of the diffusing particles. When this effect can be observed rather slightly by varying the time step size it is enormous in the case of changing the set of probabilities. To investigate this sensitivity a next test series has been performed. Now the diffusion coefficient has been hold constant but the relations between the probabilities have been modulated as presented in Table 2.

Table 2: Constant diffusion coefficients with several sets of probabilities

D	400	400	400
p_0	0.10	0.25	0.40
p	0.40	0.25	0.10
Γ	0.94	0.88	0.79

This test indicates a strong influence of the probabilities. Even though the diffusion coefficient as computed by Equation (7) is identical in all cases the resulting labyrinth factors Γ differ. Apparently a decreasing probability p causes an increasing hindrance of diffusion. To illustrate the consequences of this fact another test has been executed. For that the diffusion coefficient has been fixed constant again and the probabilities of a ballistic trajectory p_0 and of reflection p_1 have been assumed to be equal. Now the parameter p has been systematically varied in a range from 10^{-4} to 10^{-2} and the other parameters have been adapted. For this test another configuration has been used. All boundaries have been assumed to be isolated and at the initial state a square of particles has been centred on the domain. In this test are no obstacles present. Figure 9 shows the computed results at different times.

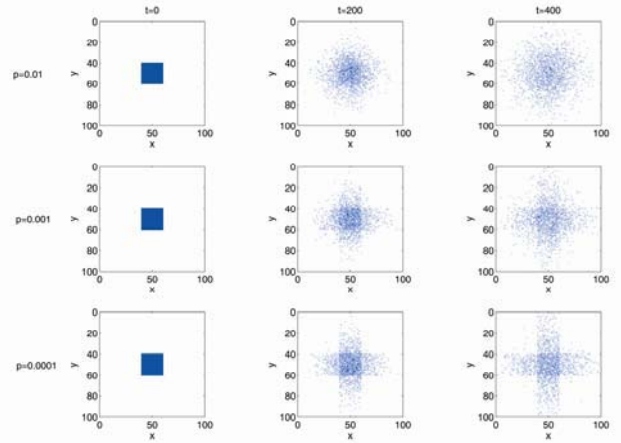


Figure 9: CA behaviour depending on probability set

While the probability $p = 10^{-2}$ leads to an isotropic diffusion in the other cases a preferred diffusing direction is identifiable. This effect becomes clear by considering the free path length of a particle. The parameter p determines the probability of a 90° deviation. In principle increasing p leads to a decreasing free path length. Figure 10 shows the comparison of two particles with different values of p .

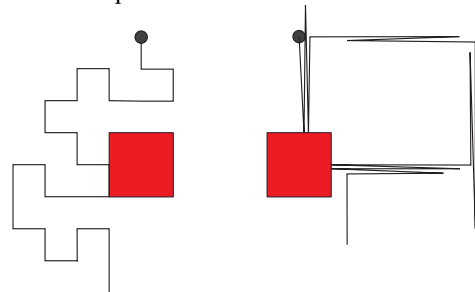


Figure 10: Particles passing obstacles

While the particle on the left with the higher value of p often changes its direction and so easily passes the obstacle, the one on the right side bounces several times against the obstacle until it finally turns and passes it

also. Since the assumption that Δx has to tend to zero in Equation (7) is not complied in this case, it has to be interpreted from a different point of view. To compare the diffusion behaviour of particles with different sets of parameters the regarded domain has to be resolved with a sufficiently fine grained net. Refining the grid leads in this case to a convergency of the results. In other words, the simulation is too far away from the critical limit in Equation (7).

To underline this, a further test has been carried out. For this the geometry of the obstacles has been changed, they became larger. In order to get comparable results their number has been decreased and so density of obstacles regarding the whole domain has not changed. In Table 3 the outcome of this test is presented.

Table 3: Refinement of the CA

D	400	400	400
p_0	0.10	0.25	0.40
p	0.40	0.25	0.10
Γ	0.83	0.80	0.77

This series confirms the thesis that the resolution of the grid has to be sufficient fine in relation to the obstacles. Applying larger obstacles in a constant grid corresponds to a reduction of the regarded area resp. increasing the spatial increment Δx . The tendency conforms to the results presented in Table 2 but the extent has significantly decreased. Finally, a series has been performed to figure out the influence of the boundary concentration c_Γ . Several simulations have been executed with different diffusion coefficients adjusted by the time step size and various boundary concentrations. Table 4 shows the outcome of these tests.

Table 4: Effects of the boundary concentrations

		D		
		200	400	600
c_Γ	0.1	0.81	0.79	0.77
	0.5	0.81	0.79	0.77
	0.7	0.81	0.79	0.77

As a result can be determined, that the sensitivity of the cellular automaton regarding the boundary concentration can be neglected.

CONCLUSION

In this paper an extension of a cellular automaton that treats diffusion processes has been developed. A short overview of the existing model has been given. After that the development of the policy extension was discussed in detail. We have exposed the influence of all concerning parameters and their technical meaning. In order to quantify the effect of obstacles the labyrinthic factor Γ has been introduced. With that special adjusted

simulation experiments have been performed to investigate the sensitivity of the cellular automaton concerning the numerical parameters. It has been observed that a sufficient resolution has to be the basis for the simulations even though the experimental results seem to be plausible. The performed investigations have shown that the developed extension of the diffusing model is considered suitable to be applied.

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Author Biographies



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WOLFGANG WIECHERT studied mathematics and computer science at the University of Bonn and obtained his diploma degree in 1985. Afterwards he joined the Department of Theoretical Biology at the University of Bonn where he got his PhD in 1991. From 1991 to 1996 he worked at the Institute of Biotechnology at the Research Center Jülich where he earned his postdoctoral lecture qualification. Since 1996 he is a professor for simulation at the Institute of Systems Engineering at the University of Siegen.