ECI Symposium Series, Volume RP5: Proceedings of 7th International Conference on Heat Exchanger Fouling and Cleaning - Challenges and Opportunities, Editors Hans Müller-Steinhagen, M. Reza Malayeri, and A. Paul Watkinson, Engineering Conferences International, Tomar, Portugal, July 1 - 6, 2007

SIMULATION OF CALCIUM PHOSPHATE DEPOSITION ON STAINLESS STEEL SURFACES: A NEW APPROACH BASED ON CELLULAR AUTOMATA

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ABSTRACT

Fouling caused by calcium phosphate upon heating is basically a crystallization/precipitation process, which starts with the formation of stable clusters of ions or molecules in a process called nucleation that occurs either in the bulk liquid or at the surface.

The cellular automata are useful tools to model complex systems of the universe. They could be considered as a good alternative to differential equations and have been used to model many physical/biological systems.

In this preliminary work, a two dimensional space was considered where the cellular automata lattice was represented as a grid of squares, with each square representing a single automaton cell.

Several situations were simulated, representing the growth of the deposit on stainless steel materials for different surface energies. The results of the simulations were compared with experimental data obtained in the laboratory.

INTRODUCTION

Milk is a complex biological fluid composed by a large number of components. To ensure the microbiological safety of the consumer's milk, it is necessary to pasteurize/sterilize the milk. Since this requires heating the milk, it promotes the build up of unwanted deposits (fouling) on the surfaces of the pasteurizers and sterilizers.

Fouling in heat exchangers is a problem to the dairy industry and costs billions of euros every year. It has been studied by many researchers, who have discussed the main variables that affect fouling. Fouling depends on several parameters such as: heat transfer method, hydraulic and thermal conditions, heat transfer surface characteristics, type and quality of milk, as well as its processing history.

At higher temperatures, calcium phosphate deposition determines the fouling rate in process equipment used for heating dairy fluids. This fouling mechanism is described by the following steps (Rosmaninho et al., 2004):

1. Formation of calcium phosphate particles in the bulk upon heating;
2. Transport of these foulant particles to the heated surface;
3. Adhesion of the particles on the heated surface;
4. Deposition of further fouling material on the top of the particles adhered to the surface.

The main objective of this work is to use cellular automata to simulate calcium phosphate deposition and compare the results with the ones obtained in previous experimental fouling tests carried out for different surface characteristics.

EXPERIMENTAL PROCEDURE

The experimental tests were carried out using simulated milk ultrafiltrate (SMUF) solutions. SMUF is a simplified milk system prepared with deionised water and appropriate amounts of reagents in order to simulate the fouling effects of the mineral components of milk.

The SMUF solutions were introduced into the thermostatic vessel within a rotating disk apparatus. The temperature was adjusted to 44 ºC. At this temperature, the solution begins to become turbid indicating the precipitation of calcium phosphate.

In milk deposits, the calcium phosphate appears in the form of several compounds, but when processing at higher temperatures and pH near 7.0, the stable calcium phosphate compound that commonly appears is hydroxyapatite.

The study reported here analyses the influence of surface energy of the fouling surface (the stainless steel plates modified with TiN thin coating, obtained by reactive sputtering on the deposition process (Rosmaninho et al., 2007). Different surfaces with a wide range of surface energy values and similar roughness and compositions were tested.

CELLULAR AUTOMATA

The concept of cellular automata was developed by John von Neumann in the 1950's (Wolfram, 1994). Driven by an interest in the general problems associated with the behavior of computing structures, von Neumann began to appreciate the complexity and performance of the human brain as a model for designing automatic computing machines. He described his system as having all of the following characteristics:

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1. An infinite plane that can be divided up into squares;
2. Each square contains a copy of the same finite automaton (the combination of the square with its automaton is called a cell);
3. A cell's neighbourhood consists of itself along with its four immediate, non-diagonal neighbors;
4. The state of a cell at time t + 1 is dependent on the state of its neighbourhood at time t and the local rule of the finite automaton in each cell;
5. The finite automaton in each cell has a start state that is the same as every other finite automaton's start state;
6. The local rule is the same for each cellular automaton and yields a consistent result.

After von Neumann developed the principles of cellular automata, other scientists began to experiment with different configurations.

The cellular automata models have their origins in the game of life of Conway. It is a simple base-rule system, involving the location of cells on a compartments array, each one verified by a computer many times until the end. If the compartment is empty, the computer moves to the next. If it is busy, the computer is directed by a base rule that points to the destiny of cell. In the game of life, the generation of a new cell, dead or an older cell, or without any alteration, is solely judged in the occupation of its neighbourhood. This is the best known abstract application of cellular automata.

The cellular automata are an array of identical, interacting cells. These models, considered abstractly, exhibit a wide variety of behaviors: self organization, chaos, pattern information and fractals.

Cellular automata can be one-dimensional, two-dimensional and three-dimensional. According to von Neumann's definition, cellular automata could be infinite in all dimensions, that is, all arrays in the above descriptions would be of infinite length in von Neumann cellular automata.

The cellular automata patterns are defined as discrete systems in space and time, where the state of one automaton is determined by a set of rules that act locally, but applied globally.

Indeed, cellular automata are grids of simple automaton connected locally. The cells on the edges of the grids could be considered in two different ways: one way is to consider the cellular automata to be infinite without edges, with cells extending off indefinitely in all directions; the other way is to treat the cells at the edges as unchanging, serving as a kind of static border. Nevertheless, a useful way is to consider the cellular automata to wrap around the edge to edge (Figure 1). Thus, the neighbor N of a cell on the top edge is the cell corresponding row at the bottom edge, and so on.

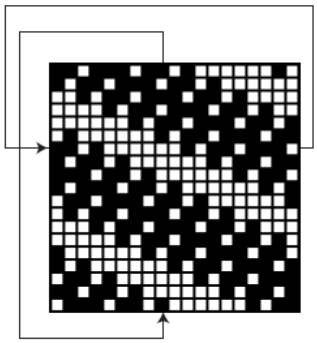

Figure 1 – Neighbourhood wrap-around

In 2-dimensional cellular automata, there are two widely-used types of neighborhoods: the von Neumann neighborhood and the Moore neighborhood. The von Neumann neighborhood, or orthogonal neighborhood, consists of a cell and its immediate neighbors to the right and left, as well as those above and below the cell (Figure 2). The Moore neighborhood, or unit cube, on the other hand, includes the cells immediately to the northwest, north, northeast, east, southeast, south, southwest, and west of the cell in question (Figure 3). There are many other types of neighborhoods in a 2-dimensional cellular automaton; some even have a circular or hexagonal shape.

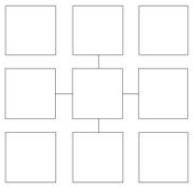

Figure 2 –von Neumann's neighborhood.

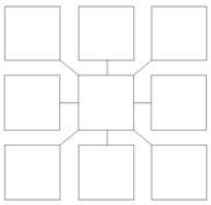

Figure 3 – Moore's neighborhood.

At each time step, a cell and its neighbors are examined to determine the state of that cell for the following time period. A rule or a set of rules is used to change the cell's state. This is referred to as the local rule or transition function. The same local rule is applied to all the cells at time t so that the state of all cells for time t + 1 is generally determined in parallel. This creates a homogeneous system in a sense that no cells have a transition function that is different from any other cell.

The cellular automata could be considered as a good alternative to differential equations and it has been used to model physical systems, like iterations between particles, creating galaxies, kinetic of molecular systems and crystal growth, as many biological systems.

Cellular automata have been used to simulate a wide range of natural processes such as turbulent fluid flow, gas diffusion, forest fires, and avalanches. It can even be used to generate pseudo-random numbers.

CELLULAR AUTOMATA AND THE DEPOSITION OF CALCIUM PHOSPHATE

The cellular automata lattice was represented as a grid of squares, with each square representing a single cellular automaton cell. The state of these squares is in the form of numerical values. For simplicity, different colours were used to represent the different states of each cell.

At each time step, the new value of each cell is determined by examining its state and the states of all neighbouring cells. For cells which lie on the edge of the cellular automata grid, the permanent state considered is the state of bulk liquid.

The new values for cells were stored in a temporary array while calculations were taking place. This occurs to ensure that all cells were using the previous states of neighbours for calculations, and not the new states. After the new values for all cells have been calculated, these values were copied to the original array.

To simulate this process using cellular automata, three possible states were created: liquid (bulk), particle and deposit. However, only two of the three states can be changed. A particle remains in bulk with the state of particle, but if this particle contacts with a particle that already has the state of the deposit, it will acquire the state of the deposit. When it gets the state of deposit, it never changes.

The element of volume of each particle was chosen according to the medium diameter of the particles that where analyzed by Coulter Counter.

Table 1 presents the main characteristics of software tool developed to simulate this process through cellular automata.

Table 1 – Main characteristics of the Software tool.

Characteristics of software tool	Description
Dimensions of the space (x, y, z)	(100.2 μm, 80.2 μm, 0.1 μm)
Dimension of element of volume (x, y, z)	0.1 μm, 0.1 μm, 0.1 μm 
Coloration state of the cell	Green - deposit; Pink - particle; Black - Bulk liquid.
Neighbourhood	Moore neighbourhood (8 neighbours)

The bulk concentration was considered constant during the deposition and the percentage of particles adhesion is different, according to the plate specificity and the characteristics of the final deposit.

THE CELLULAR AUTOMATA RULES

Rules were set to promote the movement of all particles through the bulk phase, using cellular automata principles. The rules are the transition functions defined by the local context of each cell at any given time. The rules that set the values of each cell at a moment produce a deterministic function of the current value of that cell and the values of that cell's neighbourhood. The states of all cells were transformed at time=0, 1, 2, etc. Thus, the states are determined at one instant by the states at the previous instant, applying simultaneously the rules at every cell. It should be noted that while the transition functions were applied locally, the behaviour was global, as were both the lattice structure and the timing regime.

The rules that obtain more qualified results are described as follows.

As shown in Figure 4, there are three blue squares representing the three cells which content may occupy the cell C(i,j). These possibilities are the positions: C(i+1,j-1), C(i+1, j) and C(i+1, j+1).

The first rules implemented were:

- Rule 1 - If a particle was present in position C(i+1, j-1) or C(i+1,j) or C(i+1,j+1) of the grid, it could occupy the cell C(i,j) in the next time t+1. They all had the same probability of filling the cell C(i, j);
- Rule 2 - When one of the positions C(i-1, j-1), C(i-1, j) and C(i-1, j+1) had the statute of deposit and cell C(i, j) is a particle, this cell acquired the statute of deposit.

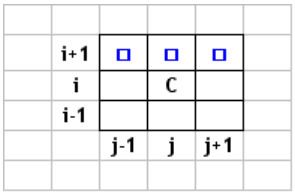

Figure 4 – Representation of the implemented rule.

To generate rules with more realistic significance, the Rule 1 was changed to consider some probability of cell C(i, j) being filled. Two values of probabilities affecting the positions of C(i+1,j-1), C(i+1,j) and C(i+1,j+1) were attained. The probability of influence from the cells C(i+1,j-1) and C(i+1,j+1) has a different value of the probability of influence from the cell C(i+1, j). These probabilities are attributed according to the deposit compaction that was expected.

The algorithm of this software tool is presented in Figure 5.

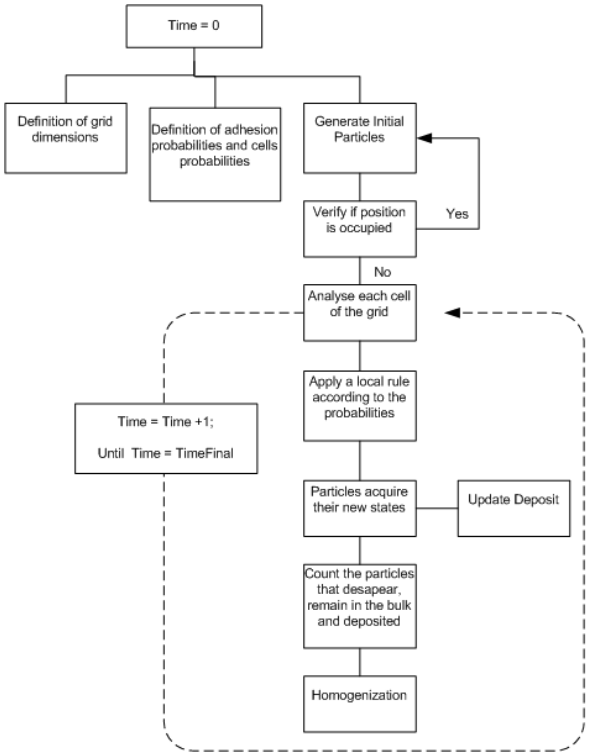

Figure 5 – Workflow of the software tool.

RESULTS AND DISCUSSION

Figure 6 shows the mass of deposit versus time obtained with the plate TiN10, both experimentally and by simulation. As can be seen, a good agreement exists between the results obtained experimentally and by simulation. The simulation data were obtained from the total cells with state deposit at several times.

Figure 7 shows, the deposit structure after 7200 seconds obtained by cellular automata.

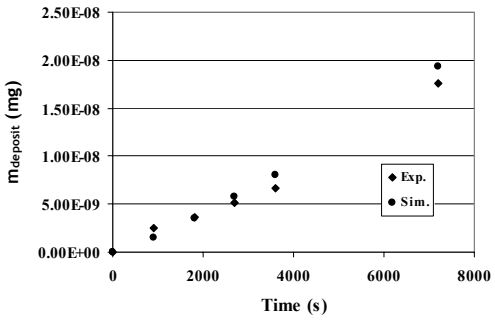

Figure 6 – Calculated versus measured mass of deposit obtained for plate the TiN10.

To achieve these results, the cell C(i,j) becomes particle with 10% of probability if one of the cells C(i+1,j+1) and C(i+1,j-1) contains already a particle. In addition the cell C(i,j) becomes also particle with a probability of 50% when the cell C(i+1,j) is a particle. This means that the vertical displacement of particles is more responsible in forming the deposit than the oblique displacement. A possible reason for this observation is the effect of agitation of the liquid in the bulk.

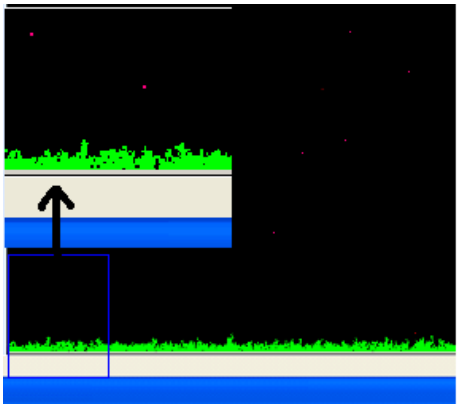

Figure 7 – Deposit structure after 7200 seconds for the plate TiN10.

In the closest layer of the plate, the cell C(i,j) becomes deposit if it is a particle and for a random probability greater than 50%.

The modification of these three probabilities and step time influence clearly the deposit structure and deposit growth.

CONCLUSIONS

The deposition of calcium phosphate is a very complex process to model. The use of computational resources can bring a significant contribution to its understanding. On the other hand, empirical data are important to improve the kind of rules that will be applied in modeling. In the present work, the basic rules that were established used the cellular automata approach. Although this paper reports preliminary work on this subject, the comparison of the experimental data with the results of the simulations provides promising results so far. Since this study is only at its initial stage, new rules, such as those describing detachment of the deposited particles, must be incorporated in the model and tested to obtain more realistic results.

AKNOWLEGMENTS

This work was supported by Fundação para a Ciência e Tecnologia under project POCTI/EQU/47654/2002.

REFERENCES

R. Rosmaninho, J. Visser, and L. Melo, 2004, Influence of the Surface Tension Components of Stainless Steel on Fouling Caused by Calcium Phosphate, *Progress in Colloid and Polymer Science*, Vol. 123, pp.203-209.

S. Wolfram, 1994, *Cellular Automata and Complexity*, Addison-Wesley Publishing Company, USA.

S. Arrhenius, 1896, On the influence of carbonic acid in the air upon the temperature of the ground, *Philos. Mag.*, Vol. 41, pp. 237-277.

R. Rosmaninho, F. Rocha, H. Müller-Steinhagen and L.F. Melo, 2007, Calcium Phosphate Fouling on TiN coated Stainless Steel Surfaces: Role of Ions and Particles, *Chem. Eng. Sci.*, accepted for publication.