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Numerical simulation of the motion of cascade vortices in the sub-surface layer

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Abstract: In the cold fusion experiment, there observed vortex patterns on a thick Pd electrode surface during long-term electrolysis in 0.1M LiOD. To understand the peculiar phenomenon, we had proposed N-cycle model, which is composed of four sequential processes including the CF reaction. In this study, numerical simulation for the analysis of the vortex patterns was performed to elucidate the relation between the vortex formation and the CF reaction. Supposing that the hypothetical particles mass evolved due to the CF reaction energy, we performed the numerical simulation using discretization method for the analysis of 3D motion of the hypothetical particles mass. The experimental results showed that the ejected particles mass from one side to another in a given rectangular box (simulate the sub-surface layer) exhibited a helical trajectory as a function of magnetic field. The traces of the ejected particles mass on another side composed vortex pattern. There has been remained more accurate simulation to examine the structure of the layer and the influence of the magnetic field.

Keyword: Computational fluid dynamics, Pd, Nuclear reaction cycle model, vortex, numerical simulation

1 Introduction

During long-term electrolysis for well annealed thick Pd rod (9.0 mmϕ) in 0.1M LiOD, vortex pattern was observed [1-2]. The morphology of the post-electrolysis electrodes revealed the two long faults without any cracks on the surface. Since the formation of this peculiar pattern of vortices can be highly plausible to the result of the Cold Fusion (CF) reaction, the precise mechanism of vortices formation must be elucidated in relation with solid state phenomenon accompanied with long-term evolution of deuterium in 0.1M LiOD. So far, an in-situ measurement of the solid state properties of dilation, resistance and electrode potential revealed that the thick Pd electrode was composed of the core structure enveloped by the sub-surface layer. The latter exhibits non-equilibrium deuterium absorption/desorption reaction. Then, N-reaction cycle model proposed [3-4] is composed of four sequential processes: in-taking and compression — triggering (the CF reaction) — scavenging. The last process: scavenging shows the traces of vortex on the electrode surface as a consequence of the process continuation. In the last papers[5-6], the vortex pattern was successfully obtained in 2D space analyzing the motion of the hypothetical particles mass by a numerical simulation method: Lattice gas cellular automata (LGCA) numerical simulation. However, there still remained ambiguity in the vortex and the CF reaction relation. In this study, because of a lack of the computational resource for 3D LGCA simulation, the other numerical simulation method, numerical simulation using discretization method, is applied for the analysis of 3D motion of the hypothetical particles mass as functions of magnetic field and matrix inhomogeneity.

2 Experimental

2.1 Long-term evolution of deuterium on thick rod Pd electrode in 0.1M LiOD

Cold fusion experiments at ambient temperatures have been conducted by electrolysis of heavy water on a Pd electrode. In Fig.1 the electrolysis

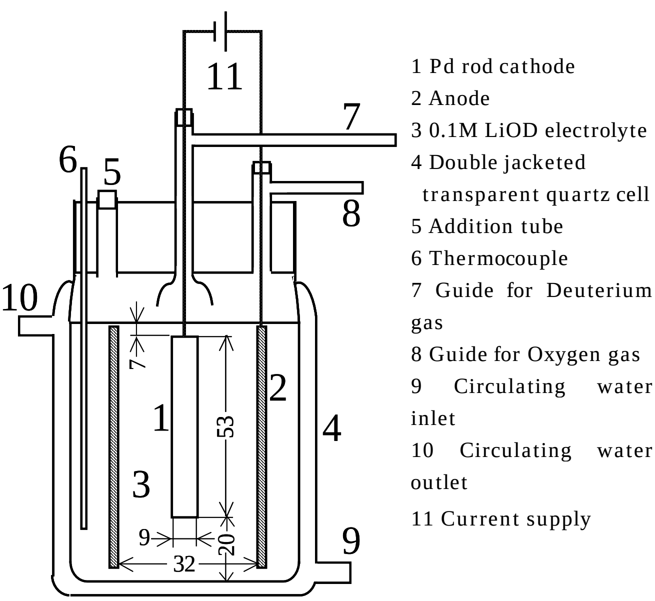


Fig.1 Schematic diagram of electrolytic cell for deuterium absorption on a Pd electrode in 0.1M LiOD.

equipment, especially the geometrical shape and arrangement of the electrode, the counter electrode (anode) and an electrolyte are shown, while the measurement systems with respect to excess heat, neutron emission, and an isothermal water bath are not drawn. Using a potentiostat (or current supply) a constant cathodic current was applied to the Pd electrode on which an evolution of deuterium gas was occurred. By continuing a state where deuterium is strongly absorbed in the Pd electrode, heat generation or emissions of neutrons or charged particles was observed. We successfully performed non-intermittent electrolysis for two and ca. six months with two experimental runs, referred to Exp.1 and Exp.2, respectively. The experimental apparatus and procedures are:

(1) Cast rod Pd electrode (2) Thicker rod Pd electrodes (Rods with 9mm and 21mm diameters [1-2]) (3) Preparatory gas phase absorption of D_2 (D/Pd = 0.36) (4) Increase in electrolysis current density in a form of stepwise (5) Temperature cycling. The experimental runs were conducted twice in 0. 1M LiOD by using the rod Pd electrodes with a diameter of 9mm referred to Exp.1[3)], and a diameter of 21mm referred to Exp.2.[1-2)]. The surface pretreatment and electrolysis conditions are shown in Table 1 and the results of neutron measurement are described elsewhere. [1-2)]

3 Results and Discussion

3.1 Experimental results of vortex for N-reaction cycle model

As shown in Table 1 the electrolysis for deuterium absorption was conducted as follows; the electrode was removed from the cell and carefully re-installed four times during which the diameter of the electrode was measured at three positions (top, middle and bottom). During 1st run the dilation at the bottom end showed 7 % while in those of 2nd- 4th runs the values at these positions approached asymptotically to 7.8-8.3 %.

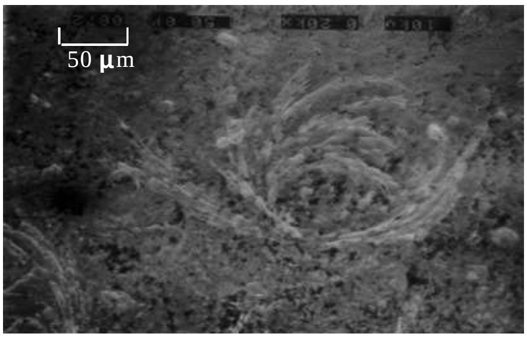
Figure 2 shows a significant morphology of a thick rod Pd electrode observed on the surface after long-term electrolysis in 0. 1M LiOD. [1-2, 7)] This peculiar pattern was named as a vortex. It is not the substance adhered on the surface, but is a material on which the pattern was deeply impressed in a shape of a ditch. This is the morphology which formation mechanism will be elucidated in the present study.

Table1 Experimental conditions of Exp.1.

Run No.	Current, $mAcm^{-2}$	Pretreatment
1st	0.05-40 40-500	Cast, 800°C anneal(10^{-6} Torr) Acid treatment
2nd	40	Polishing, Acid treatment, Evacuation, D_2 gas charge
3rd	40	Evacuation, Polishing, Acid treatment
4th	40	Evacuation, Polishing, Acid treatment

Alternately, we have investigated the microscopic structural change of Pd absorption/desorption by electrolysis as a fundamental study of deuterium absorption behavior. Although a precise description is not shown in this paper, structural change of discrimination of the sub-surface and the bulk was developed by the deformation during prolonged deuterium absorption.[8-9)] The above result with respect to the structural change of Pd must be useful in the elucidation of intake of reactant followed by compression of N-cycle model. (see Fig.3)

(a)



(b)

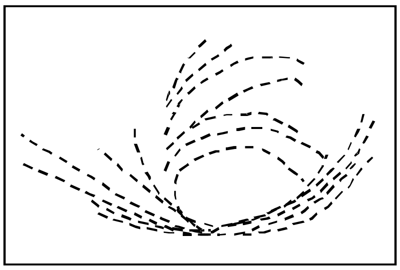


Fig.2 Vortex appeared on Pd electrode surface after long-term electrolysis in 0.1M LiOD (a), Duplicate of SEM picture (b).

3.2 N-reaction cycle model

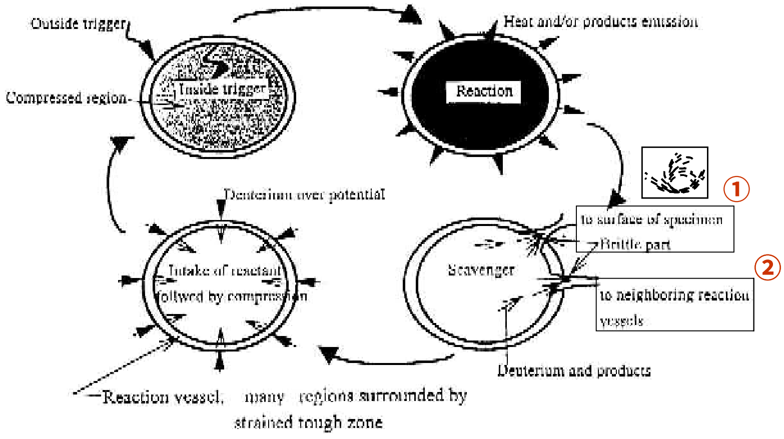


Fig.3 Schematic of nuclear reaction cycle model.

Considering that such structural changes on the electrode surface and the bulk are related with the CF reaction, it is possible to think these unusual treatments as a precursor to the CF. That is, the electrolysis performance makes the special microstructure (shown below in the simulation model), where that process is named as the intake reactant followed by compression. Next, the CF reaction could be initiated by some trigger. At this moment, in the matrixes around reaction sites the explosive energy of the CF reaction is transferred to the kinetic energy of the mobile hypothetical particles mass. In order to make the explosive energy spread over from the reaction site, the hypothetical particles mass (a group of small charged particles is considered as particles mass in this study) was assumed to be a working medium in the following simulation. Instantaneously, flow with high energy evolves and inevitably interacts with the matrix of the sub-surface layer leaving in vortices on the sample's surface (vortex shown in Fig.2).

Under such an idea, by considering the phenomena as an analogy with an energy engine (4 reciprocating cycle), N-reaction cycle model[3-4, 8)] was proposed. As schematically shown in Fig.3, it consists of 4 sequential processes: in-take and compression — trigger — reaction — scavenger where instead of the CF reaction and trigger, microstructure formation is incorporated into the successive chain and followed by scavenger. The following two key points are beneficially realized: (1) enhanced reproducibility of the experiments resides in continuation of the cycle (2) on systematic consideration the hindered factors might come to the surface. In Fig.3 the reaction vessel (indicated by double solid lines) is composed of the tough wall, which might be formed after long-term electrolysis or under repeated deuterium absorption/desorption performances. It is noted that the wall functions facile desorptive contraction/sluggish absorptive expansion.[8-9)]

For scavenger the followings are demonstrated; the in-situ measurement of the physicochemical properties of Pd-H(D) system elucidated the formation of fine nano-precipitates: $Pd\text{-}D_{2\text{-}x}$ in β-phase matrix. These precipitates assume the characteristics of non-equilibrium, hence superplasticity is often observed during their transient state. Therefore, it is envisaged that the above mentioned flow could trail through such matrix: sub-surface layer resulting in the experimentally observed vortices.

3.3 Result of Lattice Gas Cellular Automata for simulating the motion of the hypothetical particles mass in the sub-surface layer

The application of numerical simulation methods helps us to understand microscopic mechanism of the vortices formation in relation with N-cycle model. Before discussion of the numerical calculations, it is noted that there are two numerical simulation methods: LGCA (in Chapters 3.3-3.4) and discretization method (in Chapter 3.5) have been utilized in our work, whereas the goal of both methods is expected to approach toward the same conclusion (characteristics see Appendix 2). Let's focus our attention to the scavenger process after the CF reaction from a microscopic view point. The key issues are the evolution of the hypothetical

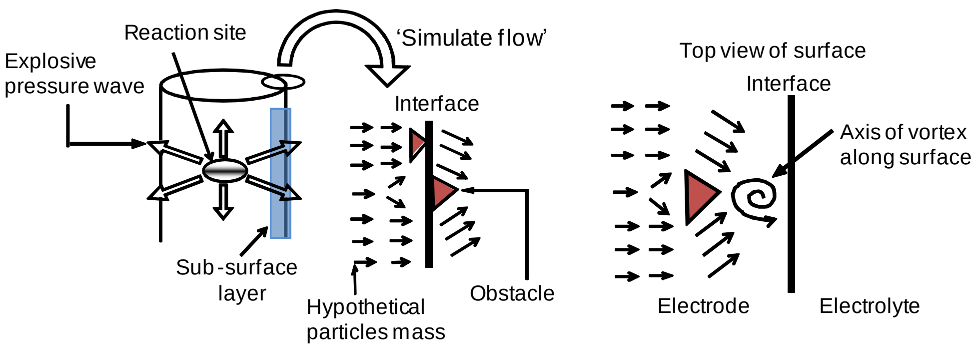


Fig.4 Perspective view of out flow of the hypothetical particles mass and vortex evolved at the interface.

particles mass with high energy, the interaction of particles mass with obstacles, and motion with magnetic field interaction through the sub-surface layer.

In the left of Fig.4, the schematic shows that the hypothetical particles mass with high energy evolves as a Scavenger process after the reaction. Subsequently, they spread outside 360˚ radial direction, and some parts reach the sub-surface layer. The condition for the radial motion will be established using a long prism crystal.[1] View from upper shows aligned vectors coincidentally rushes towards the interface as 'Simulated flow'. (see the left of Fig.4) There has been appeared simulated flow vectors normal to the electrode interface. It is easily understood for such flows to be disturbed due to the obstacles. In the right of Fig.4, it shows how evolves a vortex behind an obstacle as a result of flow disturbance. Noticeably, the axis of the vortex is along that of the cylindrical electrode.

Firstly, the results[5-6] of LGCA simulation for the vortex pattern are described. The morphological identification of the vortices has been done by comparing the 2D LGCA patterns with those experimentally obtained. The results of the simulation qualitatively well agree with the experimental patterns. By the way, as a necessary condition for this simulation, all the flows should synchronize with the occurrence of the reaction. It is tentative understanding how such flows (composed of the hypothetical particles mass) gain considerable amounts of energy. However, the fusion energy might be transferred to deuterons, and then the hypothetical particles mass near the reaction sites becomes a high pressure. Thus, the motion explosively occurs with surrounding 360˚ of the reaction sites.

Secondly, obstacles might be embedded beneath the surface due to structural inhomogeneity. The precipitates such as PdO, Li_2O and LiD, and/or vacancy cluster can correspond to actual structural inhomogeneity. In the right of Fig.4, under the flow of the hypothetical particles mass the vortex was evolved behind an obstacle.

More advanced LGCA simulations showed that the cascade of two identical rectangular domains containing each a plate evolved an individual vortex behind each plate.[6] This suggests the one-to-one correspondence between a simple obstacle and a vortex evolved by the flow. However, this is the case when two obstacles regularly aligned to generate corresponding vortices. In as received Pd such obstacles surely distribute in the matrixes and hence vortices make the different patterns corresponding to the distribution. Then, next research should be directed toward more complicated cases to simulate the motion of the hypothetical particles mass. This research still continues.

3.4 Structure and properties of the sub-surface layer deduced from Scavenger process of N-cycle model

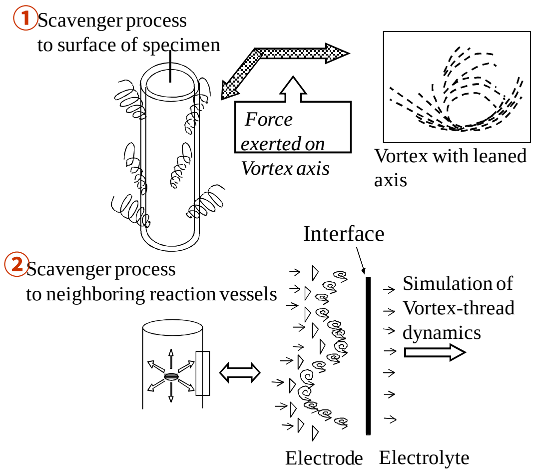


Fig.5 Schematics of vortex with leaned axis and vortex thread during Scavenger process: motion of the hypothetical particles mass from vessel to surface and from a vessel to a neighboring one.

In Scavenger of Fig.3, there were naturally assumed alternative two mechanisms of the hypothetical particles mass motions as a result of N-cycle model examination. One is ① of Fig.3: to electrode surface and another ② of Fig.3: to a neighboring reaction vessel. Two characteristic morphologies of the surface and the underneath microstructure are discussed vide infra, in relation with the appearances of the Scavenger process. In Fig.5① it shows the locus of the occasional particle flow on the Pd surface (correspond to Fig.3 ①), which was identical to the experimentally observed vortex pattern. By comparing the vortex pattern with the experimentally obtained one the axis of the motion leaned due to the interface's magnetic field.[10] On the other hand, Fig.5② shows the continuous flow of the hypothetical particles mass from a vessel to a neighboring one (corresponds

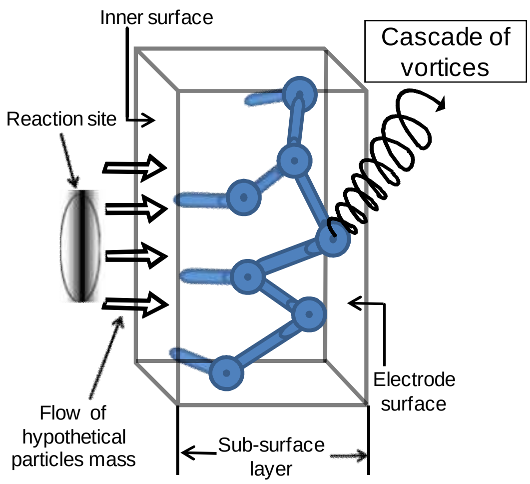


Fig.6 Motion of the hypothetical particles mass and evolved cascade vortices in sub-surface layer.

to Fig.3②). In the right of Fi.g5② many vortices are evolved behind obstacles and a cascade of vortices is seen. It has been suspected that the hypothetical particles mass also has the vortex pattern at the electrode surface. Hence, a reasonable inference leads conclude us that the vortex occurred occasionally, while the cascade vortices, vortex-thread, moves underneath the electrode surface. This view might not be inconsistent with the irregularity of sub-surface layer under an annealing at 1100℃.[11] Therefore, it is claimed that the appearances of the vortices are strongly concerned with the kinetics of the mass transfer phenomenon underneath the surface.

In Fig.6 the structure of 3D sub-surface layer is schematically shown, where the explosive energy is transferred from the reaction site. There appeared to move the hypothetical particles mass through the thick piping. The vortex threads themselves (see Fig.5②) may enable to move instead of the hypothetical particles mass. However, there still exists ambiguity on how large scale of vortices evolved (actually those diameters range to c.a. 80μm). Then it necessitates to present accurate model with respect to energy and mass transfer in the sub-surface layer. Momentum and mass transportation in the sub-surface layer might be accomplished in the following ways; it holds forward transportation rate and backward one equal implying an equilibrium state, and otherwise net transportation rate with either direction continues implying a non-equilibrium state. (Fig.7) In the latter case, as shown in Fig.7 the net flow encounters by Rayleigh–Taylor's instability resulting in an evolution of vortices.

Thus, it has become apparent that the electrode surface involving sub-surface layer significantly influences the motion of particles by electro-magnetic field and barriers (e.g. wall and obstacle). Since N-cycle model predicted that the hypothetical particles mass explosively spouted out from the reaction site and reached to the area of sub-surface layer, it is required to analyze the

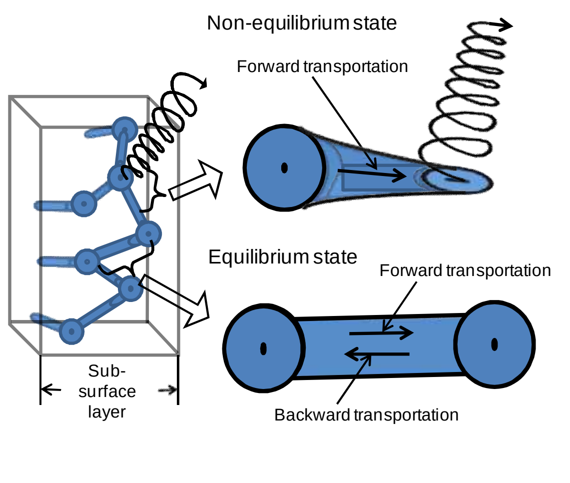


Fig.7 Transportation phenomenon in sub-surface layer and evolution of vortex.

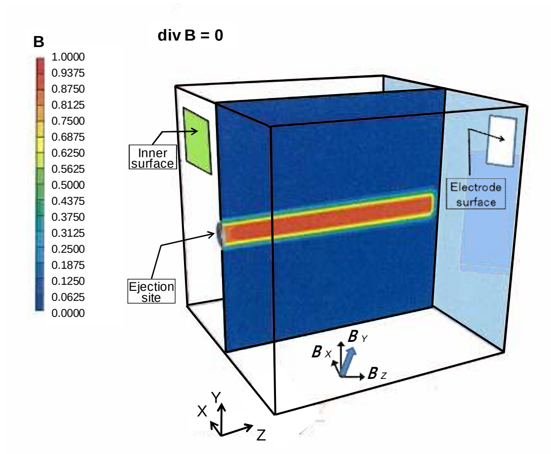


Fig.8 Magnetic field distribution on the ejection site in the sub-surface layer.

motion with magnetic field interaction within the sub-surface layer.

3.5 Motion of the hypothetical particles mass under the influence of magnetic field

We analyzed the motion of the hypothetical particles mass through the sub-surface layer using discretization method (refer Appendix 1) under the influence of magnetic field. As mentioned before, the hypothetical particles mass possessing initial velocity v_0 normal to the inner surface moves through the sub-surface layer. For simulation, the interaction with the magnetic field was incorporated where its distribution is assumed, as shown in Fig.8. It expands like the cylinder on the ejection site. The higher values concentrate along the centerline of the cylinder, while it abruptly attenuates at the periphery of the column. Due to such magnetic field distribution the hypothetical particles mass moves helically confined within the column.

The ejected particles mass trajectory draws helical streamlines as shown in Fig.9. The source of the ejection is set at the inner surface where

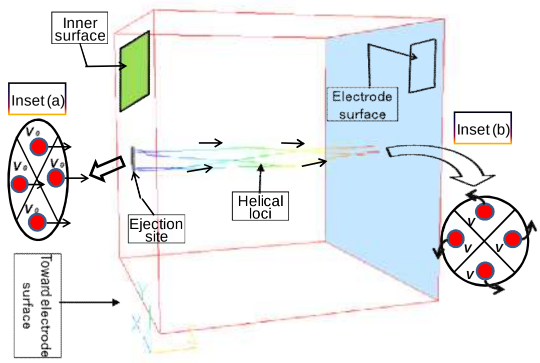


Fig.9 Time evolution of streamlines of the particles mass ejected at the inner surface toward the electrode surface in the sub-surface layer. Inset (a) shows four particles possessing initial velocity v_0 on the quadru poles of the ejection disk and that of (b) shows reached particles possessing velocity v.

four particles mass were artificially placed as shown in the left side of the simulating 3D space. In the figure, each particles mass exhibits a helical streamline reaching at the surface of the electrode. On the electrode four particles mass coincidently move outside where each particles mass left the corresponding loci. Inspecting the trajectory of the particles mass on the electrode surface, the vector of each particles mass composes curvature with concentric as shown in the inset (b). Supposedly, the shape may exhibit some energetic particles ejected from the sub-surface layer. Thus, the hypothetical particles mass moves 3D space of the sub-surface layer presenting vortex due to the interaction with magnetic field.

Although obstacle's distribution is not taken into, as preliminary, the sources of the energetic particles mass are located at the inner surface from which the flow evolved by the ejection as schematically shown in the inset (a) of Fig.9.

4 Conclusion

In this study, the numerical simulation using discretization method was applied to analyze the motion of the hypothetical particles mass. For simulation the structure and magnetic field distribution in the sub-surface layer were incorporated, and the time evolution of the particles' motion exhibited helical trajectory ejected to the electrode surface. Such moving particles mass with high energy was attributable to the CF reaction energy, as explained using N-cycle reaction model. The traces of ejected particles mass composed the vortex pattern.

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Appendix 1

Kinetic equation of the motion of the hypothetical charged particle (negative unit charge) under magnetic field is shown,

$$\mathbf{F} = q\mathbf{V} \times \mathbf{B}$$

where **F** indicates force on charged particle, q electric charge, **V** velocity and **B** magnetic field strength. Velocity and position of charged particle change with time,

$$\mathbf{V} = \mathbf{V}^{old} + \mathbf{F}/\mathbf{m} \cdot \Delta \mathbf{t}$$

$$\mathbf{X} = \mathbf{X}^{old} + \mathbf{V}\Delta \mathbf{t}$$

where **X** and **V** indicate position and velocity with advanced time $\mathbf{t} + \Delta \mathbf{t}$, $\mathbf{V}^{old}$ and $\mathbf{X}^{old}$ velocity and position at given time **t**, **m** mass, $\Delta \mathbf{t}$ time increment. The followings are initial conditions for **X** and **V**,

$$\mathbf{V_0} = (0, 0, v_0),\ \mathbf{t} = 0$$

$$\mathbf{X_0} = (0, 0, 0),\ \mathbf{t} = 0.$$

Appendix 2

Scenario and characteristics of the numerical simulations of the hypothetical particles mass's motion in the subsurface layer.

	Cellular automata	Discretization method
principle low of motion	momentum and mass conservation	Maxwell's equation, fluid equation
component particle	fluid element (microscopic)	ejected particles mass flow possessing charge (macroscopic)
driving force, B.C.	pressure difference between inflow and outflow; 2D rectangular domain, incompressible fluid	Electro-magnetic field;3D hexahedron, incompressible fluid
Advance-ment	cascade of vortices: vortex thread, interaction with obstacles, curved wall, various physical constants	realization of precise electro-magnetic field, evaluation of complex matrix
superiority	incorporation of obstacle's interaction, begin with no budget	easy calculation of complex fluid (ex. 3D and matrix)
semi goal	integrated understanding in relation with N-cycle model	