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Initial Value Problem Formulation of 3D Time Domain Boundary Element Method

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A time domain boundary element method (TDBEM) gives us another possibility of time domain microwave simulations in addition to a finite difference time domain (FDTD) method. In particular, the TDBEM has good advantages in analysis of coupling problems with charged particle motion such as in a particle accelerator. However, it is known that time domain microwave simulations in the particle accelerator by the conventional TDBEM often encounter numerical instability and inaccuracy owing to its bad matrix property. To avoid the numerical instability and inaccuracy caused by the conventional open boundary problem formulation of the TDBEM, an initial value problem formulation of 3D TDBEM is presented in this paper.

***Index Terms*— Microwave propagation, Particle accelerators, Moment methods, Numerical simulation**

I. INTRODUCTION

A time domain boundary element method (TDBEM) provides us another possibility of time domain simulations of microwave phenomena [1]-[4] in addition to a finite difference time domain (FDTD) method. The TDBEM has advantages in open boundary problems, treatments of slightly curved boundary objects, coupled problems with charged particles, etc. compared with the FDTD method. In particular, the coupled problem with charged particles such as analysis of wake fields in a particle accelerator is one of the most suitable applications of the TDBEM owing to its surface meshing. However, a treatment of infinite length structure of the particle accelerator is a very difficult subject in the TDBEM, therefore, a numerical model of a finite length accelerator tube with thin thickness has been used mainly in conventional works [3],[4]. Then, the microwave simulation by the TDBEM was often numerically unstable in a long range simulation owing to the thin thickness structure of the numerical model. To improve this problem of the numerical stability, an initial value problem formulation of the TDBEM was presented for axis-symmetric two-dimensional problems [5]. In general, two-dimensional TDBEM can be used in only restricted applications. In this paper, the initial value problem formulation (IVPF) of the TDBEM is extended to three-dimensional cases, and it is shown that the numerical stability is effectively improved from the conventional formulation.

II. II. TIME DOMAIN EFIE/MFIE AND TDBEM

It is known that time domain electromagnetic fields, $\mathbf{E}(t,\mathbf{x})$, $\mathbf{B}(t,\mathbf{x})$, in a domain V can be expressed using electromagnetic fields on the domain surface $S=\partial V$ in the following surface integral equation [3],[4];

$$\begin{aligned}\mathbf{E}(t,\mathbf{x}) &= \mathbf{E}_{ext}(t,\mathbf{x}) + \frac{1}{4\pi}\int_S \left\{ \frac{\mathbf{n}'\times\dot{\mathbf{B}}(t',\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \right\} dS' \\ &+ \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right)(\mathbf{E}(t',\mathbf{x}')\cdot\mathbf{n}') \right\} dS' \\ &+ \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right)\times(\mathbf{E}(t',\mathbf{x}')\times\mathbf{n}') \right\} dS', \end{aligned} \tag{1}$$

$$\begin{aligned}\mathbf{B}(t,\mathbf{x}) &= \mathbf{B}_{ext}(t,\mathbf{x}) + \frac{1}{4\pi}\int_S \left\{ \frac{\dot{\mathbf{E}}(t',\mathbf{x}')\times\mathbf{n}'}{|\mathbf{x}-\mathbf{x}'|} \right\} dS' \\ &+ \frac{1}{4\pi}\int_S \left\{ \left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right)\times(\mathbf{n}'\times\mathbf{B}(t',\mathbf{x}')) \right\} dS' \\ &+ \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right)(\mathbf{n}'\cdot\mathbf{B}(t',\mathbf{x}')) \right\} dS', \end{aligned} \tag{2}$$

which are the time domain versions of a well-known EFIE and MFIE in a frequency domain [6],[7]. $\mathbf{E}_{\mathrm{ext}}(t,\mathbf{x})$ and $\mathbf{B}_{\mathrm{ext}}(t,\mathbf{x})$ are externally applied electric and magnetic fields, respectively, the retarded time $t\,'$ is defined by $t'=t-|\mathbf{x}-\mathbf{x}'|/c$, c is the velocity of the light and $\mathbf{n}$ is a unit normal vector on the surface. To discretize Eqs.(1) and (2) in time and the surface, we obtain a matrix equation containing many matrices (Fig.1), which should be solved as the 3D TDBEM. Unknown vectors in the matrix equation are two components of a surface current and charge densities $\mathbf{K}$, σ, which correspond to $\mathbf{n}\times\mathbf{B}$ and $\mathbf{n}\cdot\mathbf{E}$ on the surface, respectively. Owing to the retarded time property of Eqs.(1) and (2), unknowns at different time steps are independent each other. Then, if we assume that the boundary S is a perfectly electric conductor (PEC) throughout, (2) results in the following very simple form;

$$\begin{aligned}\mathbf{B}(t,\mathbf{x}) &= \mathbf{B}_{ext}(t,\mathbf{x}) \\ &+ \frac{1}{4\pi}\int_S \left\{ \left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right)\times(\mathbf{n}'\times\mathbf{B}(t',\mathbf{x}')) \right\} dS'. \end{aligned} \tag{2)'$$

which was used in the conventional TDBEM.

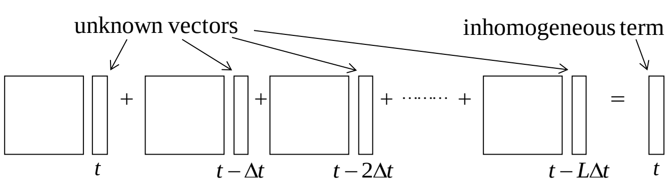
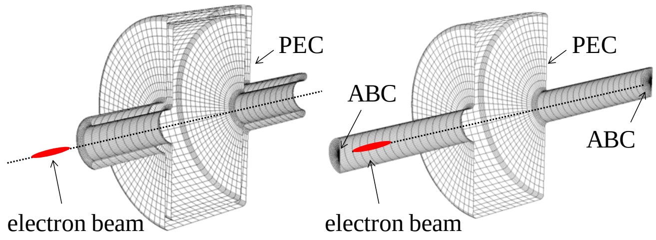


Fig. 1. Structure of matrix equation of TDBEM



(a) open boundary thin double layer model (b) closed domain model

Fig.2. Numerical model of a part of particle accelerator tube

III. Treatment of Infinite Length Structure of Particle Accelerator in TDBEM

In derivation of the integral equations (1) and (2), it is assumed that there are no surface current and charge density at the initial time. To satisfy these conditions and realize the simulation of wake fields by a finite length numerical model, an open boundary problem formulation using a thin double layer numerical model with a torus topology (Fig.2(a)) was used in conventional works. Then, it was assumed that the electron beam was located at sufficiently far upstream distance from the finite length accelerator tube at the initial time to satisfy the conditions of no surface current and charge density on the domain surface. In this formulation, the domain boundary is PEC throughout, therefore, the simplified formulation (2)' can be used. However, the conventional method using the numerical model of Fig.2(a) had some difficulties, a bad matrix property caused by the thin double layer structure of the numerical model, an instability caused by an interior resonance in the long range simulation, and large calculation size owing to the double layer structure of the numerical model.

IV. Initial Value Problem Formulation of 3D TDBEM

To improve these difficulties, which are caused by the open boundary problem formulation (2)' and thin double layer numerical model (Fig.2(a)), the initial value problem formulation of the TDBEM, which allows us to use the numerical model with a closed domain structure (Fig.2(b)), was proposed for axis-symmetric two-dimensional cases. However, the TDBEM with the assumption of axis-symmetric system can be used only in restricted applications. In this paper, the initial value formulation of the TDBEM is expanded to three-dimensional cases. For the case that there are non-zero surface current and charge densities on the domain surface at the initial time $t = t_0$, Eqs.(1) and (2) are generalized as follows [5]

$$
\begin{aligned}
\mathbf{E}(t,\mathbf{x}) = {} & \mathbf{E}_{ext}(t,\mathbf{x}) + \frac{1}{4\pi}\int_S \left\{ \frac{\mathbf{n}'\times\dot{\mathbf{B}}(t',\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \right\} dS' \\
& + \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \left(\mathbf{E}(t',\mathbf{x}')\cdot\mathbf{n}'\right) \right\} dS' \\
& + \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \times \left(\mathbf{E}(t',\mathbf{x}')\times\mathbf{n}'\right) \right\} dS' \\
& + \frac{1}{4\pi}\int_{V_0} \left(\left(\dot{\mathbf{E}}(t',\mathbf{x}') + \frac{\partial \mathbf{E}(t',\mathbf{x}')}{\partial r'} \right) \frac{|\mathbf{x}-\mathbf{x}'|}{c} + \mathbf{E}(t',\mathbf{x}') \right) dV',
\end{aligned}
\tag{3}
$$

$$
\begin{aligned}
\mathbf{B}(t,\mathbf{x}) = {} & \mathbf{B}_{ext}(t,\mathbf{x}) + \frac{1}{4\pi}\int_S \left\{ \frac{\dot{\mathbf{E}}(t',\mathbf{x}')\times\mathbf{n}'}{|\mathbf{x}-\mathbf{x}'|} \right\} dS' \\
& + \frac{1}{4\pi}\int_S \left\{ \left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \times \left(\mathbf{n}'\times\mathbf{B}(t',\mathbf{x}')\right) \right\} dS' \\
& + \frac{1}{4\pi}\int_S \left\{ -\left(\frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^3} + \frac{(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\frac{\partial}{c\partial t} \right) \left(\mathbf{n}'\cdot\mathbf{B}(t',\mathbf{x}')\right) \right\} dS' \\
& + \frac{1}{4\pi}\int_{V_0} \left(\left(\dot{\mathbf{B}}(t',\mathbf{x}') + \frac{\partial \mathbf{B}(t',\mathbf{x}')}{\partial r'} \right) \frac{|\mathbf{x}-\mathbf{x}'|}{c} + \mathbf{B}(t',\mathbf{x}') \right) dV',
\end{aligned}
\tag{4}
$$

Differences in (3) and (4) from the conventional integral equations (1) and (2) are only the existences of the fifth terms, which are contributions of volume integral on V_0 at the initial time, that is, a bottom super-surface of the 4D time-space region Ω of Fig.3. The normal component of magnetic field $\mathbf{B}\cdot\mathbf{n}$ and the tangential component of electric field $\mathbf{E}\times\mathbf{n}$ disappear on the PEC boundary and exist only on the absorbing boundary condition (ABC) virtual surface. The fifth terms in (3) and (4) are superposed on the inhomogeneous term in practical calculations, and the time domain simulation based on (3) and (4) is carried out in the same manner as that of Fig.1. A detail structure of the matrix equation corresponding to (3) and (4) is indicated in Fig.4. Unknown vectors are composed of two tangential components of magnetic field B_s, B_t and a normal component of electric field E_n on the PEC boundary. Contribution from the virtual surface with the ABC is summarized as the second inhomogeneous term. (see Fig.4)

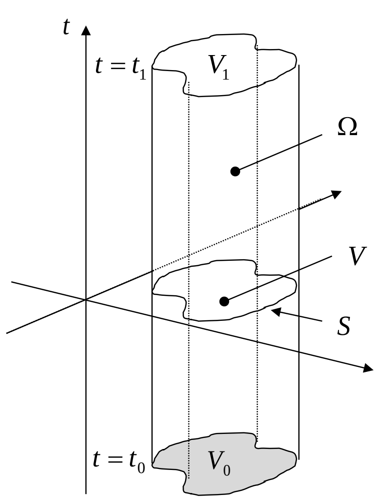


Fig.3. 4D time-space volume between time t_0 and t_1

$$
\begin{bmatrix} G^0_{BBss} & G^0_{BBst} & \mathbf{0} \\ G^0_{BBts} & G^0_{BBtt} & \mathbf{0} \\ G^0_{EBns} & G^0_{EBnt} & G^0_{EBnn} \end{bmatrix}
\underbrace{\begin{bmatrix} B_s^{\,k} \\ B_t^{\,k} \\ E_n^{\,k} \end{bmatrix}}_{\text{unknowns at present time step}}
=
\overbrace{\begin{bmatrix} B_{ext\,s}^{\,k} \\ B_{ext\,t}^{\,k} \\ E_{ext\,n}^{\,k} \end{bmatrix}}^{\text{inhomogeneous term caused by electron beam self-fields}}
- \sum_{l=1}^{L} \left\{ \begin{bmatrix} G^l_{BBss} & G^l_{BBst} & \mathbf{0} \\ G^l_{BBts} & G^l_{BBtt} & \mathbf{0} \\ G^l_{EBns} & G^l_{EBnt} & G^l_{EBnn} \end{bmatrix}
\underbrace{\begin{bmatrix} B_s^{\,k-l} \\ B_t^{\,k-l} \\ E_n^{\,k-l} \end{bmatrix}}_{\text{unknowns at previous time steps}} \right\}
+ \overbrace{\begin{bmatrix} B_{ABC\,s}^{\,k} \\ B_{ABC\,t}^{\,k} \\ E_{ABC\,n}^{\,k} \end{bmatrix}}^{\text{2nd inhomogeneous term contributed from ABC}}
$$

Fig. 4. Configuration of matrix equation of TDBEM with IVPF

V. Numerical Examples

The first numerical example is a numerical model of a pill-box cavity in the particle accelerator (Fig.2). The tube inside radius is 2cm, radius and longitudinal length of the cavity part are 12cm both, and it is assumed that the electron beam with 1.5cm length Gaussian distribution travels on the axis with the light velocity *c*. Owing to axis-symmetric structure of this model, transient electromagnetic fields (wake fields) induced by the electron beam (Fig.5) can be simulated by the 2D TDBEM and the axis-symmetric 2D FDTD method as well. Fig.6 indicates comparison of so-called longitudinal wake potential $W(s)$ defined by,

$$W(s)=\frac{e}{Q}\int_{-\infty}^{\infty}\mathbf{E}\left(r=0,z,t=\frac{(z+s)}{|\mathbf{v}|}\right)dz \tag{5}$$

which means total energy loss of a virtual particle traveling at distance *s* behind the original electron beam.(see Fig.5) It is found that three methods, the 2D-FDTD method, the 2D-TDBEM with the conventional open boundary formulation and the presented method (3D), show good agreements each others. Then, conventional 2D-TDBEM needs the discretization of 200 divisions at least for rotational direction around the axis to obtain the sufficiently good agreement with the 2D-FDTD method owing to the bad matrix property caused by the thin double layer numerical model of Fig.2(a). On the other hand, the presented method, the TDBEM with IVPF needs 40 divisions at most.

The second example is numerical models of the slightly curved accelerator tube with rectangular cross-section indicated in Fig.7. The electron beam with 1.5cm length Gaussian distribution travels on the center axis of the tube. The vertical and horizontal size of the rectangular cross-section are 2cm and 8cm, respectively. The longitudinal length of the curved section has 18 degree angle with the curvature radius 1.6m. It is easily imagined that the FDTD grid generation of this numerical model is not easy, and the 3D TDBEM surface meshing is much more suitable. The closed model for the presented IVF and the open boundary model for the conventional formulation are shown in Fig.7(a) and (b), respectively. In Fig.7(a), upstream straight section is additionally extended to smoothly begin the electron beam motion, compared with Fig.7(b). In addition, an infinitely spread parallel plate model (Fig.7(c)(i)) is considered here, which gives us a approximately semi-analytical solution by using a method of infinite vertical series image charges. (see Fig.7(c)(ii)) A time domain behaviors of two tangential components of the magnetic field B_s and B_t, which correspond to the induced surface currents, on the observation lines in Fig.7 are indicated in Fig.8 for the longitudinal current component, and in Fig.9 for the rotational current component. In this case, the longitudinal surface current of Fig.8 is the main component, and therefore Fig.8 is plotted in 50 times bigger scale than those of Fig.9. Fig.8(a), (b) and (c) indicate simulation results by the presented method, the conventional 3D TDBEM and the image charge method, respectively. We can find sufficiently good agreements between these three simulations. Fig.9(a), (b) and (c) are also drawn as same manner as in Fig.8, then Fig.(b) is plotted in 10 times bigger scale than the other two plots. Owing to semi-static calculation based on the image charge method in the numerical model of Fig.7(c), the rotational current components, which are created by inductive behavior of the electromagnetic fields during the curved motion of the electron beam, show different behavior in Fig.9(a) and (c). In particular, the conventional TDBEM simulation of Fig.9(b) contains serious unnatural and unphysical oscillations, which come from inaccuracy caused by the bad matrix property owing to the thin double layer model, although Fig.9(b) is made by finer meshes by using 10 times bigger memory (350GB) than that of Fig.9(a). Calculation times are 300 min. by a single node, 340 min. by four parallel nodes and 330 min. by single node on a supercomputer HITACHI SR16000 for Fig.7(a), (b) and (c), respectively.

VI. Summary

In this paper, the initial value problem formulation of 3D TDBEM has been presented. The proposed method is applied to analysis of the wake fields in the particle accelerator. It is shown that the proposed method provides us stable simulations of the time domain microwave phenomena than those of the conventional formulation. In particular, the improvement of the stability allows us to use coarse meshes, which means that effective memory reduction is achieved by the initial value problem formulation.

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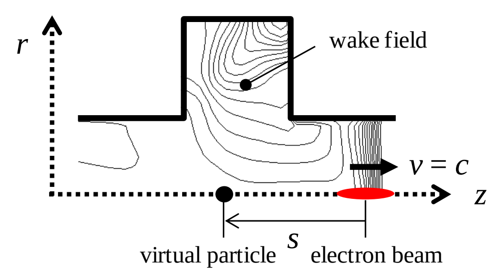

Fig. 5. Virtual particle travelling at distance *s* behind electron beam

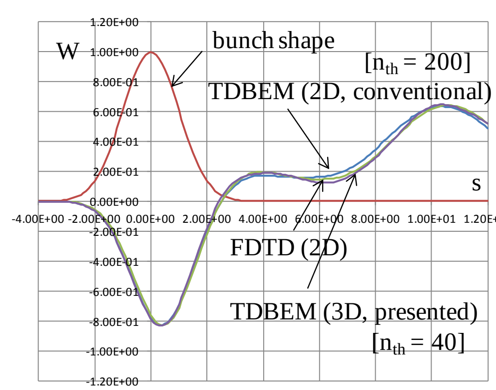

Fig. 6. Comparison of wake potential calculated by 2D-FDTD, conventional 2D-TDBEM and presented methods

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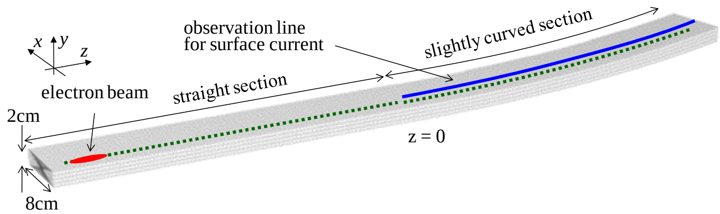


Fig. 7 (a) . Numerical model of slightly curved accelerator tube (closed domain model)

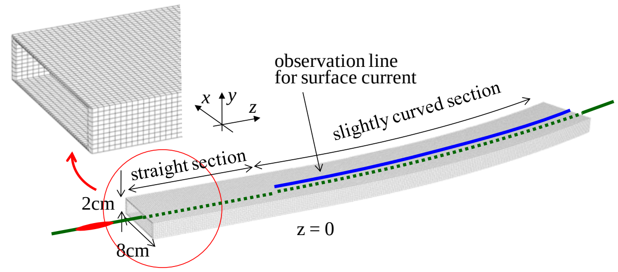
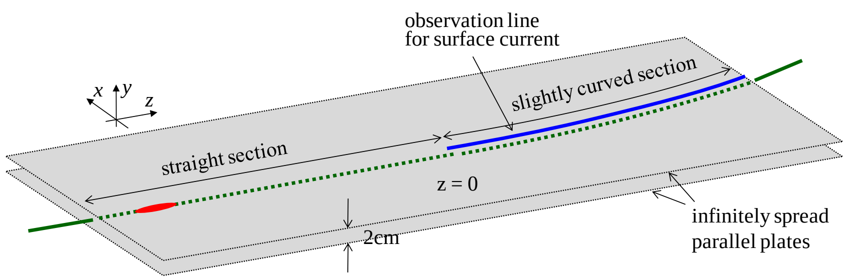
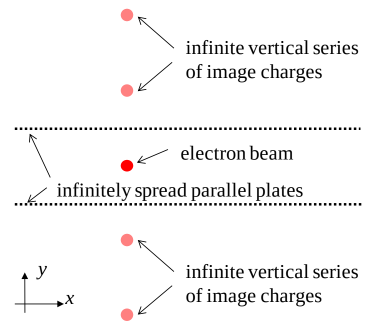


Fig. 7 (b) . Numerical model of slightly curved accelerator tube (thin double layer open boundary model)

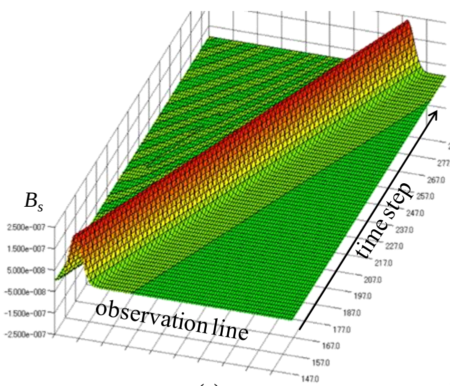


(i)

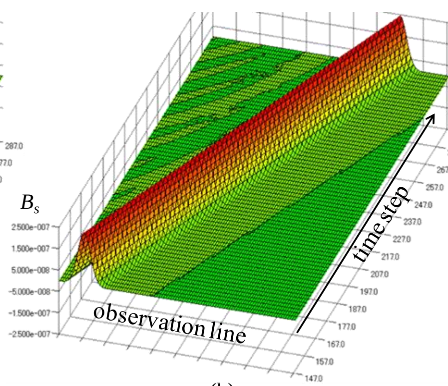


(ii)

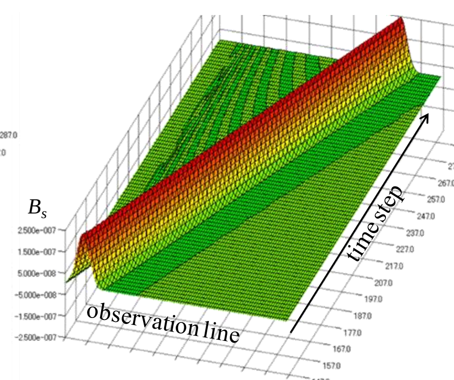
Fig. 7 (c) . Numerical model of infinitely spread parallel plates (i) and method of infinite series image charges (ii)



(a)

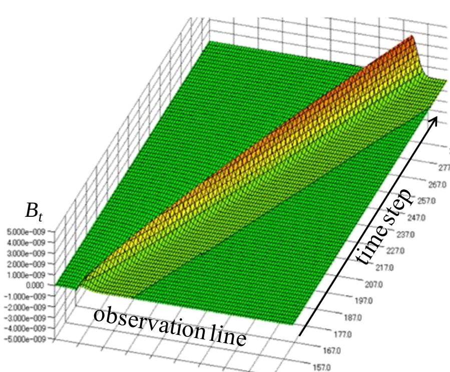


(b)

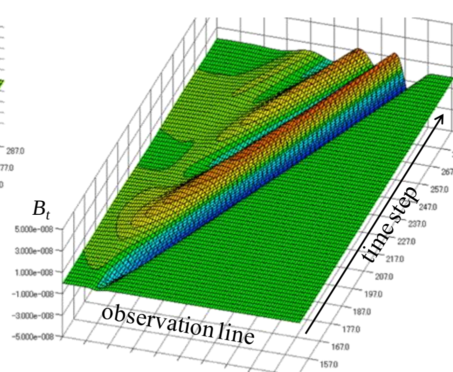


(c)

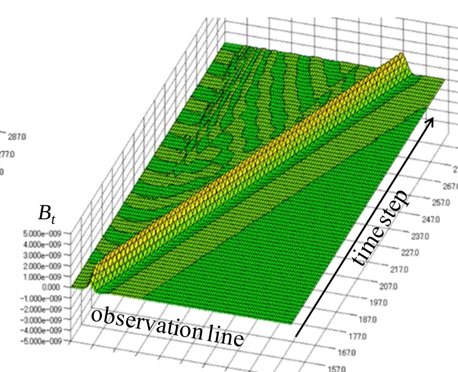
Fig. 8. Time domain behavior of longitudinal component of induced surface current



(a)



(b)



(c)

Fig. 9. Time domain behavior of rotational component of induced surface current