A Numerical Calculation Method Advantageous for Complex Boundary Problems
-An Application to the Pulse Discharge Sintering Process-

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A numerical method based on the Method of Fundamental Solutions coupling with the Fourier transformation is presented. The advantage of the new method is demonstrated by solving the nonlinear partial differential equations, which are derived for the simulation of the pulse discharged sintering process to obtain the electric potential and temperature profiles in the system. In this problem, the delta function is revealed at the interface between the different component materials, graphite mold/punch and powder sample. The properties change there as a step function. The efficiency of the method is indicated with regard to solving the problems including the discontinuous functions as a whole without dividing the system to two different material parts. The calculation results showed that the temperature in the system is controlled by the heat conductance from the punch, where a large Joule heat evolution is observed without depending on the sample properties. The calculated temperature in the sample is relatively uniform.

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1. Introduction

In material developments, it is seldom to handle only single or uniform materials. Several materials are usually combined, instead. In case of such composite materials, the physical properties show discontinuity at the junction part. This kind of discontinuity is treated as boundary conditions in computer simulations by the conventional methods such as finite element method (FEM) and boundary element method (BEM). The system must be separated by the boundary, since discontinuous functions in the system cannot be incorporated directly in these numerical simulation techniques. There is a constraint at the interface to solve the governing equations. Temperature, for example, is generally constrained to be connected continuously there. When several materials are combined in the complex manner, boundary conditions become complex and the calculation procedure becomes complicated in the conventional numerical simulation techniques.

The Method of the Fundamental Solutions (MFS) has recently progressed as a grid-free numerical method for, particularly, the case of nonregular geometrical-boundary conditions.\textsuperscript{1-3} It is considered as one of the collocation methods for the integral equation derived from the differential equation,\textsuperscript{4} including a convolution as volume integral. MFS has, however, a problem in this convolution. The boundary-domain element method\textsuperscript{5} is usually used for it, but the reduction of the dimension, which is an advantage of the boundary element method, cannot be employed efficiently. One of the authors has proposed an efficient method to solve the convolution in MFS.\textsuperscript{6} That is to move the calculation domain to the frequency space by the Fourier transformation. The convolution can be obtained simply as an algebraic product in the frequency space. Another advantage of using the frequency space is that the delta function after the derivative in the real space is treated as a continuous function in the frequency space. The representation as a constant function in the frequency space will make it possible to solve the whole domain including the discontinuous section as a unit-domain.

This method is, in this paper, applied to analysis of electric potential and temperature distributions in the pulse discharge sintering (PDS) process as a first step, even though the method is efficient in more complicated systems. In this process it is important to keep the temperature in a powder sample uniform during the PDS process for producing high quality products. The sample is placed in a graphite mold, which has different thermal and electric conductivities from the powder sample. While the physical properties change at the interface between the sample and the mold as a step function, i.e. the delta function in the derivative, is easily incorporated in the present numerical method and the whole system is easily treated as a unique calculation domain in the frequency space.

This paper describes the outline of the method in Section 2, the model of the PDS process in Section 3, and the numerical calculation results of temperature and electric potential distributions in Section 4. Section 5 is for conclusion.

2. Numerical Calculation Procedure

Basic equations necessary for analyzing the PDS process are the Poisson equation and thermal conduction equation. These equations are written in the following general formula including a linear differential term $Au(x)$ and an inhomogeneous/nonlinear term $f(x)$, in which $A$ is a constant coefficient linear partial differential operator, $u(x)$ is an unknown function to be solved, and $x$ represents coordinates.

$$Au(x) = f(x) + \sum_{S} S_{g}(x - x_{g}).$$ \hspace{1cm} (1)

Source term $S_{g}$ in this equation was introduced to represent the boundary conditions. Here the $S_{g}$ values are given by a
delta function at point \(x_5\), in the same way as MFS. This additional term is called a source in MFS. (It is often called as a charge, though it is not necessary to be a real electric charge. We don’t use the latter terminology here to avoid confusion.)

From the Fourier transformation of eq. (1), Fourier transformed form of the unknown function \(u(x)\), \(\hat{u}(\xi)\), can be obtained formally in the frequency space as

\[
\hat{u}(\xi) = \frac{\hat{f}(\xi)}{A(i\xi)} + \sum \left[ \frac{1}{(2\pi)^n} \frac{1}{A(i\xi)} \exp(-i\xi \cdot x_5) \right] S_5,
\]

where \(n\) is dimension of the space and \(A(i\xi)\) is called as total symbol of the homogeneous equation corresponding to eq. (1) in pseudo-differential operators theory. Since the boundary conditions are built in this equation, it is not necessary to divide the system into several different-material domains. This means that the partial derivative equations are solved as a whole. If the function \(f(x)\) contains the unknown function \(u(x)\), \(u(x)\) can be obtained by the successive substitution method. Fast Fourier Transformation (FFT) can be used to achieve a high performance in the numerical calculations by dividing the system into the same size in the real space under the periodic boundary conditions.

The source intensities are obtained by solving simultaneous linear equations derived from the boundary conditions in the similar way as used in MFS. When function value \(u(x)\) is known at point \(x_B\) as \(\varphi(x_B)\) on a boundary (Dirichlet boundary problem), Fourier inverse transformation of eq. (2) gives

\[
u(x_B) = \varphi(x_B) = \int_\Omega \hat{f}(\xi) \exp(i\xi \cdot x_B) d\xi + \sum s \left[ \int_\Omega \frac{1}{(2\pi)^n} \frac{1}{A(i\xi)} \exp(-i\xi \cdot x_5) \exp(i\xi \cdot x_B) d\xi \right] S_5,
\]

When a slope/derivative of function \(u(x)\) at \(x_B\) is given (Neumann boundary problem), two-point difference approximation gives

\[
\varphi(x_B) = \frac{\partial u}{\partial x} \bigg|_{x=x_B} = \frac{u(x_N) - u(x_B)}{\Delta x} = \int_\Omega \hat{f}(\xi) \exp(i\xi \cdot x_N) - \exp(i\xi \cdot x_B) d\xi + \sum s \left[ \int_\Omega \frac{1}{(2\pi)^n} \frac{1}{A(i\xi)} \exp(-i\xi \cdot x_5) \frac{\exp(i\xi \cdot x_N) - \exp(i\xi \cdot x_B)}{\Delta x} d\xi \right] S_5.
\]

Point \(x_N\) is, here, one point away from boundary point \(x_B\) by \(\Delta x\). Robin boundary problem is easily treated in the same way as the Neumann boundary problem as described in the above.

When each boundary point \(x_B\) is one-to-one correspondence to the source point \(x_5\), number of unknown values \(S_5\) is equal to that of boundary condition formulas. Thus, sources \(S_5\) are determined by solving eq. (3) and eq. (4) as simultaneous linear equations. The different types of boundary conditions are solved at once; it is not necessary to solve each boundary condition in the different way. Numerical quadratures in \([\cdots]\) of eq. (3) and eq. (4) are performed by the Trapezoidal rule in order to use the same manner as used in the numerical quadrature in FFT.

Discretization in this method is similar to the sampling theory in the signal processing, in which the function is expressed as a delta function on a sampling point. When the sources are on the grid point, calculation efficiency can be improved by the rectangle approximation for the sources.

3. Model of Pulse Discharge Sintering

The PDS apparatus consists of graphite mold/punch and powder sample as shown in Fig. 1. The electric current passes through these graphite and powder between two electrodes.

3.1 Governing Equations

3.1.1 Electric potential distribution

The basic equation for electric potential \(\varphi\) distribution is
the following Poisson equation with additional source terms in this method.
\[
\text{div}(\kappa \text{ grad } \phi) = \sum_S S_S \delta(x - x_S).
\]  
(5)

Substituting electric conductivity \(\kappa\), which is a function of \(x\), by constant term \(\kappa_0\) and variable one \(\kappa'\) as
\[
\kappa(x) = \kappa_0 + \kappa'(x),
\]  
(6)
eq (5) becomes to have a linear part in the left side and an inhomogeneous part in the right side as follows.
\[
\Delta \phi = -\frac{1}{\kappa_0} \text{div}(\kappa' \text{ grad } \phi) + \frac{1}{\kappa_0} \sum_S S_S \delta(x - x_S).
\]  
(7)

This equation is related to eq. (1) in the cylindrical coordinates, \((r, z)\), as follows.
\[
A = \frac{\partial^2}{\partial r^2} + \frac{\partial^2}{\partial z^2},
\]  
(8)

\[
u(x) = \phi(r, z),
\]  
(9)

\[
f(x) = \frac{1}{r} \frac{\partial \phi}{\partial r} - \frac{\kappa'}{\kappa_0} \left( \frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial z^2} \right) + \frac{1}{\kappa_0} \left( \frac{\partial \kappa' \phi}{\partial r} + \frac{\partial \kappa' \phi}{\partial z} \right).
\]  
(10)

Boundary conditions are given on the electrodes and mold walls as
\[
\phi = E_{\text{Bottom electrode}} \quad \text{and} \quad \phi = E_{\text{Top electrode}},
\]  
(11)

\[
\left. \frac{\partial \phi}{\partial r} \right|_{\text{mold wall (side)}} = 0 \quad \text{and} \quad \left. \frac{\partial \phi}{\partial z} \right|_{\text{mold wall (top or bottom)}} = 0.
\]  
(12)

\(\kappa_0\) can be any value formally, but it must be \(|\kappa'| < |\kappa_0|\) to make the numerical solution be converged. Although the calculation range of the \(r\)-direction can be limited from 0 to \(R\) from the symmetry, we adopted \(-R \leq r \leq R\) in order to use FFT. Periodic boundary conditions are automatically satisfied in this calculation range.

Since Fourier transformed Laplace operator has the zero value at the origin, it is impossible to define the inverse element. The similar procedure as the Green function theory is, here, introduced for avoiding the integration at the pole; the following formula of inverse operator \(A^{-1}\) is used.
\[
\frac{1}{A(i\xi, i\eta)} \equiv \frac{1}{2} \left[ \frac{1}{-\xi^2 - \eta^2 + i\varepsilon} + \frac{1}{-\xi^2 - \eta^2 - i\varepsilon} \right].
\]  
(13)

In the numerical computations, \(\varepsilon = 10^{-20}\) is used. Although there is no restriction basis in this assumption at present, it is judged by the numerical computation results.

### 3.1.2 Temperature distribution

In the PDS method, the sample is heated by Joule heat due to the current, which is calculated from the potential as \(\kappa \text{ grad } \phi\). Joule heat \(q\) at each place is, therefore, given by
\[
q = \kappa \text{ grad } \phi^2.
\]  
(14)
The temperature distribution as a function of time \(t\) is obtained by solving the heat conduction equation
\[
c_p \rho \frac{\partial T}{\partial t} = \text{div} (\lambda \text{ grad } T) + q + \sum_S S_S \delta(x - x_S),
\]  
(15)

where \(c_p\) is heat capacity, \(\rho\) density, and \(\lambda\) thermal conductivity, all of which are functions of \(x\) and expressed by the constant and variable terms as eq. (6). Equation (15) becomes in the cylindrical coordinates, \((r, z)\)
\[
AT(r, z) = f(r, z) + \frac{\alpha}{\alpha_0 \kappa} \sum_S S_S \delta(r - r_S) \delta(z - z_S),
\]  
(16)

where thermal diffusivity \(\alpha\) is expressed as
\[
\alpha = \frac{\lambda}{c_p \rho}, \quad \alpha = \alpha_0 + \alpha'.
\]  
(17)

A and \(f(r, z)\) are
\[
A = \frac{1}{\alpha_0 \Delta t} - \frac{\partial^2}{\partial r^2} - \frac{\partial^2}{\partial z^2},
\]  
(18)

\[
f(r, z) = \frac{1}{\alpha_0 \Delta t} T_{r-\Delta t} + \frac{\alpha'}{\alpha_0} \left( \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right) + \frac{\alpha}{\alpha_0 \kappa} \left( \frac{\partial \lambda}{\partial r} \frac{\partial T}{\partial r} + \frac{\partial \lambda}{\partial z} \frac{\partial T}{\partial z} \right) + \frac{\alpha}{\alpha_0 \kappa} q.
\]  
(19)

where \(\Delta t\) is a time step for the calculation of the time development.

The electrodes are cooled by a coolant, and the other walls are cooled by the radiation loss expressed by the Stefan-Boltzmann law. Therefore, the boundary conditions are,
\[
\lambda \left. \frac{\partial T}{\partial z} \right|_{\text{on electrodes}} = h(T_B - T_\infty),
\]  
(20)

\[
\lambda \left. \frac{\partial T}{\partial r} \right|_{\text{mold wall (side)}} = \sigma (T_B^4 - T_\infty^4),
\]  
(21)

\[
\lambda \left. \frac{\partial T}{\partial z} \right|_{\text{mold wall (top or bottom)}} = \sigma (T_B^4 - T_\infty^4),
\]  
(21)

where \(h\) is over-all heat transfer coefficient from the electrode to the coolant, \(\sigma\) the Stefan-Boltzmann constant, \(T_B\) temperature at the boundary, and \(T_\infty\) temperature of the surroundings.

### 3.2 Calculation domain

The calculation domain for solving the governing equations for the PDS process is shown in Fig. 2. The domain consists of two parts, graphite (electrode, punch, and mold) and powder sample. It was discretized to grid points of \(64 \times 64\) with interval equal to 1 mm. The boundary and source points were collocated on the grid points. The boundary surface in Fig. 2 corresponds to the mold surface. The outside of the boundary is imaginary space used in the present method like as MFS.

### 3.3 Material properties

The physical properties of graphite and copper powder change during the sintering process. Fang et al.\(^7\) reported density, electric resistivity and thermal diffusivity as a function of the temperature during the PDS process of copper powder. We used their data shown in Figs. 3(a)-(c). These properties of copper powder change mainly by densitization due to sintering than by temperature itself. While there was no actual measurement of the constant-pressure heat ca-
pacity of copper powder, the literature data\textsuperscript{9)} were used with the measured porosity in the calculations.

4. Results and Discussion

4.1 Electric potential distribution

The electric potential distribution obtained in two cases under the uniform temperature distribution at 303 K is shown in Fig. 4; one is with the copper powder as a sample and another is with graphite itself as a sample for comparison. The potential and current distributions along the \( z \)-axis are shown in Fig. 5 and Fig. 6. In these figures the calculation results obtained by the conventional differential method with the successive over-relaxation method (SOR method) are shown for comparison.\textsuperscript{9)} In these calculations, electric potentials \( E \) of \( \pm 0.5 \) V were applied on the two electrodes. Electric conductivity of the copper powder at \( T = 303 \) K was used for the standard physical-property value \( k_0 \). The calculation results by the present method are, of course, well consistent with those by the conventional method.

In the case that all parts are made by graphite, it is found from the potential distribution in Fig. 4 that currents spread from the electrode to the inside of the mold. In the case of the copper powder sample, the currents are concentrated into the sample, which has the higher electric conductivity than graphite.

Since \( \kappa' \) changes in a step function at the interface between copper powder and graphite, the space differentials, \( \partial \kappa'/\partial r \) and \( \partial \kappa'/\partial z \), in eq. (10) could not be discretized at the interface by the conventional techniques like FEM and BEM; the boundary must be counted separately from other calculation domains in these techniques. Analytically, these derivatives are the delta function and given by measure. In the present calculation technique, the delta function is approximated with a rectangle,\textsuperscript{10} By using this technique, dissociation of the boundary from the other uniform part is not necessary.

With the operation procedure used here, it was possible to carry out numerical computations for the whole system as a unique calculation domain.

There is no rule in arrangement of source points in this calculation. When these source points were collocated just on the boundary surface, no correct behavior at four corners of the powder sample was obtained. The Neumann boundary

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Fig. 2 Calculation domain. Gray square and its surroundings are a sample and a graphite mold/punch, respectively.

Fig. 3 Physical properties of copper, sintering copper powder and graphite during the PDS process (measured by Fang et al.\textsuperscript{5}) (a) Density, (b) Electric conductivity, (c) Thermal diffusivity.
Fig. 4 Potential distribution in the calculated domain at 303 K. Samples (located in the inner square) are (a) graphite and (b) copper powder.

(a) Graphite

(b) Copper powder

Fig. 5 Potential profiles in the z-direction at r = 0 with the results by the differential method for comparison. Samples are (a) graphite and (b) copper powder.

(a) Graphite

(b) Copper powder

Fig. 6 Current density profiles in the z-direction at r = 0 with the results by the differential method for comparison. Samples are (a) graphite and (b) copper powder.
condition is satisfied even if the incorrect sources are placed at these four corners. Therefore, the search of the correct solution may have become to the wrong direction. This is improved by selecting a suitable position for a source. It should be noted here one more weak point that it is difficult to calculate the potential distribution inside the insulator, \( \kappa = 0 \).

### 4.2 Temperature distribution

The temperature change due to Joule heat in the system makes the physical properties change and the potential distribution change. Heat evolution is balanced with heat transfer from the electrodes cooled by the coolant and radiation from the mold surface. Distributions of electric potential \( \phi \), heat generation \( q \), and temperature \( T \) at the steady state are shown in Fig. 7 and Fig. 8 for two cases, using graphite and copper powder as a sample. Potentials \( E \) on the two electrodes are set to be \( \pm 0.4 \) and \( \pm 0.3 \) V in the cases of graphite and copper powder samples, respectively. The standard physical-property values \( \kappa_0 \), \( \alpha_0 \), \( \rho_0 \), and \( C_0 \) used are \( 2 \times 10^3 \Omega^{-1} \text{m}^{-1}, \ 1.17 \times 10^{-4} \text{m}^2 \text{s}^{-1}, \ 8.97 \times 10^3 \text{kgm}^{-3} \) and \( 385 \text{Jkg}^{-1} \text{K}^{-1} \), respectively. These values are those at room temperature except \( \kappa_0 \). In the calculation with the copper powder sample, \( \kappa_0 \) was reset to \( \kappa \) at the center at every time step. The number of iteration at each time step was 20, by which good convergence was obtained. Calculation was done with a time step \( \Delta t = 1 \text{s} \) to achieve the steady state.

The current flows from the narrow part (punch) to the large part (mold). For this reason, large potential slope is observed in the punch near the electrodes and large heat generation is observed in the punch near the electrodes as shown in Fig. 7. Two peaks of the heat generation are observed on the electrode because of concentration of the current at the edges. Since the electrodes are forced to be cooled, large temperature slope are also observed near the electrodes. In the case of the graphite sample, potential distribution is similar to that at the room temperature shown in Fig. 4(a), since graphite has small temperature dependence in electric and thermal conductivities. Temperature increased uniformly at the whole part of the system.

The electric conductivity of copper powder is 12 times larger than that of graphite at room temperature, though the ratio is increased to 280 times around 660 K. For this reason, large influence of \( \kappa / \partial r \) is observed for the potential distribution at high temperature. The current is more concentrated in the sintered copper powder than the graphite mold. Although the temperature slope is large near the graphite electrode, it

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**Fig. 7** Calculation results of the PDS process for the sample filled with graphite at \( t = 500 \text{s} \) (\( E = \pm 0.4 \text{V}, k = \lambda_{\text{graphite}}/(0.05 \text{m}) \)). (a) Potential profile, (b) Profile of heat production, (c) Temperature profile.

**Fig. 8** Calculation results of the PDS process for the sample filled with copper powder at \( t = 500 \text{s} \) (\( E = \pm 0.3 \text{V}, k = \lambda_{\text{graphite}}/(0.05 \text{m}) \)). (a) Potential profile, (b) Profile of heat production, (c) Temperature profile.
is small in the sample part (sintered copper powder) due to the high thermal conductivity of the sintered copper powder and no heat generation in the high electric conductivity part. Therefore, the comparatively uniform temperature distribution in the sample part was obtained in this calculation model.

It is worth to note that the present method can give the good stability in the time evolution in solving the linear equation problem, since time and space are not coupled. If the governing equation is a constant coefficient heat conduction equation, the time step can be determined without regard to the grid size in the space. In the case where the sample part is constituted from graphite, calculation was stabilized even with a time step of $\Delta t = 10$ s.

5. Conclusion

A newly developed calculation method based on the MFS coupling with the Fourier transformation was described. Several advantages were shown with simulation of the PDS process. Step and delta functions, which appear in the basic equation to express the interface between graphite (mold and punch) and powder sample in PDS, are, in this method, handled easily using Fourier transformation. It was possible to calculate temperature and electric potential distributions in the system including the different materials without dividing the system into several domains of the same materials.

The temperature profiles in the two cases in which sample part is filled with graphite or copper powder were shown as a demonstration of the present method. There was a little heat generation in the sample part in both cases. Joule heat is mainly generated near the electrode and temperature in the sample increased relatively uniformly with a little dependence on sample properties in this calculation model.

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REFERENCES

9) The calculation was done with the same grid points as the present new method in the ordinary domain for the same boundary value problem.
10) When the derivative of $x$ at the interface was approximated by two-point difference, potential slope from the interface to the inside of the copper powder was overestimated.