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Basic Concept and Application of Differential Operator in Time and Space by Orthogonal Collocation Finite Elements Method

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Abstract

The aim of this paper is to spread the basic concept and the application of orthogonal collocation finite elements method (OCFEM) to the field of engineering and science. OCFEM is based on Weierstraßs polynomial approximation theorem. In the formulation of PDE as strong form by OCFEM, the differential operator represented by matrix in time and space is used for the translation of PDE to algebraic equation. This paper explains the concept of matrix representation method of the differential operator in time and space, the coordinate transformation matrix based on the partial derivative of composite function and integration of element (for example, Consumption rate) or element boundary (for example, Flux) by using Gauss Legendre [i]integration. On the other hand, this paper presents the formulation of advection-diffusion-reaction equation (PDE) as initial boundary value problem, which is Biofilm model, by differential operator of OCFEM.

Keywords: Orthogonal Collocation Finite Elements Method, Differential Operator, Time and Space, Coordinate Transformation Matrix, Biofilm Model, Advective Diffusive Equation, PDE, Initial Boundary Value Problem

Introduction

The basic concept of the orthogonal collocation finite element method (OCFEM), which is the subject of this paper, is based on orthogonal collocation method (OCM), which is considered to be a kind of weighted residual method. Since it seems important for understanding OCFEM to describe the historical evolution of the orthogonal collocation method, we will explain it using the literature (1) of B.A. Finlayson. In addition, since there is a risk of confusion about the interpretation of the basic concepts in the spectral collocation method, differential quadrature method [(2)], and spectral element method, which are said to be the same concept as the orthogonal collocation method, we will not explain them here. The basic concept of differential operators (matrix) is used for the explanation.

The orthogonal collocation method was first advanced by Lanczos (1938, 1956), Clenshaw, Norton (1963), Norton (1964), and Wright (1964) used the Chebyshev polynomial to solve the initial value problem of ordinary differential equations as an application example. This implicitly indicates that the orthogonal collocation method could be used to solve the initial value problem of the evolution equation. Villadesen and Stewart (1967) [(3)] applied the orthogonal collocation method to the boundary value problem, and chose a collocation orthogonal polynomial (N+1st order polynomial) as a trial function that satisfies the boundary conditions and in which the roots of the Nth order orthogonal polynomial give collocations. On the other hand, the solution is simplified by directly calculating the solution of the boundary value problem by giving it as the values of the solution at the orthogonal collocation (the root of the orthogonal polynomial), rather than finding the solution as a coefficient of the polynomial. The entire problem is replaced by a series of matrix equations, which can be easily solved by a computer. In addition, an accurate quadrature equation is used (an orthogonal polynomial with weights $w = 1-x^2$ in the Jacobi polynomial: also called the Lobatto polynomial), which makes it possible to integrate using the solution at the orthogonal collocation. If the root of the Legendre polynomial used in this paper is chosen as the orthogonal collocation, it can be seen that the numerical integration point of Gauss Legendre's numerical integral (Gauss's numerical integral) is the same as the orthogonal collocation, so it can be almost accurately integrated [(4)].

The orthogonal collocation method has been applied mainly to the field of chemical engineering (advection-diffusion-reaction equations) [(5) ~ (11)]. Subsequent research on the orthogonal collocation method was directed toward the finite element of the orthogonal collocation method, and the research was mainly led by Finlayson et al. [(5)(6)]. In order to know the past research and development direction of Finlayson et al.'s collocation method on finite element (OCFE) [(5) ~ (11)], the outline of the contents of the paper by Finlayson et al. is itemized and Ohkubo's current idea of orthogonal collocation finite element method (OCFEM)) [(12) ~ (16)] will also be explained.

① Finlayson et al. [(5) ~ (11)] formulated the basic equations on the internal collocations in the elements and the boundary condition equations (Directre conditions, Neumann conditions, and mixed boundary conditions) on the external collocations on the boundary by the orthogonal collocation method, and used the mixed method in the collocation method of ②.

② The selection method of polynomials as a trial function of OCFEM is a mixed method that uses a trial function that does not satisfy both the basic equations and the boundary conditions, and finds a solution that satisfies both the boundary conditions and the PDE. In the case of one-dimensional spaces, the same method is used in OCFEM by Mikami et al. [17] and Finlayson et al. However, in order to facilitate the procedure of element connection in the mixed method for two-dimensional problem, it is necessary to create a differential operator (matrix) that can be derived from the Lagrange interpolation formula for two-dimensional space, and connect the elements at external collocations according to the numbering of finite elements. It will be possible to further extend to three-dimensional space.

③ In the case of a two-dimensional space, the representation of the interpolation equation using orthogonal collocations as a function is two-dimensional Lagrange interpolation formula. When the Hermite interpolation equation is used as in Finlayson et al, the concept of a differential operator cannot be constructed. At each point of four corner collocation, least square method is used to put together 4 boundary condition in corner collocation to one conditional equation.

④ Finlayson et al. focused only on rectangular elements as two-dimensional element shapes. In Ohkubo's OCFEM, a coordinate transformation matrix from the local coordinate system to the global coordinate system is created. The coordinate transformation matrix is a point-in-point transformation in its strong form, and it uses the law of partial derivatives of composite functions to convert partial derivatives from the local coordinate system to the global coordinate system.

⑤ Differential operators (matrices) in space and time by OCFEM are not limited to abstract concepts, but can be used to create concrete differential operators (matrices) for various orthogonal polynomials [18] Jacobi, Legendre, Tschebyscheff, Laguerre $(0,\infty)$, Hermite $(-\infty,\infty)$. I believe that this suggests the possibility of applying differential operators (matrices) in OCFEM to physics.

Based on these ideas, we have introduced the foundations of past researchers leading up to OCFEM and Ohkubo's ideas. Differential operators (matrices), coordinate transformation matrices, and the area integration within an element (Gauss numerical integration) and the line integration of element boundaries (Gauss numerical integration) in OCFEM are described in each section. In order to formulate PDE’s (advective diffusive reaction equation) by orthogonal collocation finite element method (OCFEM), we performed an analysis using differential operators (matrices) in space and time, which is the basic concept of the OCFEM.

This paper presents the results of the OCFEM formulation and numerical calculation of two-region biofilm model of the two-substrate limitation advection-diffusion-reaction equation which is Biofilm model.

Basic Concept of OCFEM

The orthogonal collocation finite element method (OCFEM) is a method that uses the orthogonal collocation method, which is said to be one of the weighted residual methods, on finite elements. In the general finite element method, the Galerkin method is used as the weighted residual method, which uses the same weight function as the trial function, but the orthogonal collocation method uses Dirac's delta function. In a strong-form differential equation, it means that the residual is zero at the orthogonal collocations. This can be expressed mathematically by the following formula.

The spatial two-dimensional linear partial differential equation is expressed by the following equations (1) and (2).

$$\dot{u} = L(u) \quad \text{: basic equation} \tag{1}$$

$$B(u) = 0 \quad \text{: boundary condition} \tag{2}$$

L, B is a linear partial differential operator

Integrating the basic equation by multiplying Dirac's delta function at the internal collocation q and the boundary condition by multiplying Dirac's delta function at the external collocation r yields Equations (3) and (4), resulting in conditional equations (5) and (6) in which the residuals are zero at the orthogonal collocation in the original basic equations (1) and boundary conditions (2).

$$\iint_e (\dot{u} - L(u))\delta(x - x_q)\delta(y - y_q)dxdy = 0 \tag{3}$$

$$\iint_b B(u)\delta(x - x_r)\delta(y - y_r)dxdy = 0 \tag{4}$$

$$\dot{u}_q - L(u_q) = 0 \tag{5}$$

$$B(u_r) = 0 \tag{6}$$

Ultimately, the orthogonal collocation method can formulate into an equation that the residual is zero at the orthogonal collocation by directly substituting the polynomial approximation and the partial derivative approximation of the polynomial in a strong form of partial differential equation. This implies Weierstraßs theorem of polynomial approximation and the approximation of partial derivatives of polynomials, and it is thought that they converge uniformly as the order of polynomials approximating the unknown function to be found is increased [4]. In the orthogonal collocation method, the Lagrange interpolation equation using the solution at the orthogonal collocation is used. In other words, it comes down to finding the solution at the orthogonal collocation instead of finding the coefficient of the polynomial assuming that the residual at the orthogonal collocation of the polynomial is zero, but by defining the differential operator (matrix) of partial derivatives [13], it is possible to easily translate partial differential equations into algebraic equations. The differential operators (matrices) for one-dimensional orthogonal polynomials can be calculated by the method of Hasegawa et al. [19] which calculate differential operators (matrices) with high numerical accuracy even in numerical calculations by differentiating the Lagrange interpolation equations. A two-dimensional differential operator can be created using a one-dimensional differential operator (the derivative of the coefficients of the Lagrange interpolation formula), and it can also be extended to three dimensions. In order to explain the relationship between Weierstraßs theorem of polynomial approximation and the differential operator of the orthogonal finite element method, we will consider a general one-dimensional polynomial.

Let u be the dependent variable and x be the independent variable of space. Again, emphasis is on Weierstraßs concept of polynomial approximation, in which a function is represented by a polynomial, and as the degree increases, the polynomial uniformly converges to a function. Equations (7) and (8) show the polynomial and the polynomial approximation u_i in x_i, respectively.

$$u = \sum_{j=1}^{N+2} a_{j-1} x^{j-1} = a_0 + a_1 x + a_2 x^2 + \cdots\cdots + a_N x^N + a_{N+1} x^{N+1} \tag{7}$$

$$u_i = \sum_{j=1}^{N+2} a_{j-1} x_i^{j-1} = a_0 + a_1 x_i + a_2 x_i^2 + \cdots\cdots + a_N x_i^N + a_{N+1} x_i^{N+1} \tag{8}$$

This is possible by using Lagrange’s the interpolation formula for orthogonal collocation, which is to express a polynomial that is a continuous function with discrete values, and to obtain a polynomial from discrete values. It shows that the discretization of continuous functions and polynomial representation (continuous functions) are equivalent. Lagrange interpolation at orthogonal collocations is used as a method of discretizing polynomials, and it can be seen that the differential operator (matrix) of OCFEM, which will be described later, is the coefficient for solving the Lagrange interpolation equation.

In the case of OCFEM, where there is a discontinuity at a certain point, it can be handled. Suppose that a region is divided into m elements piecewise. At a discontinuous point, the discontinuous part can be represented by subtracting the discontinuous amount at the boundary between the elements and taking the balance (performed by the external collocation of elements).

In determining the coefficients of a polynomial (as a continuous function) or determining the dependent variable u_i in the independent variable x_i (discretization), the position of the root x_i of the Nth order orthogonal polynomial of the element interval (e.g., the Nth order Sifted Legendre polynomial) is important. It is important that the differential operator is calculated by the value of this orthogonal collocation (the root of the orthogonal polynomial), and it is necessary to consider the meaning of the weight function with respect to the orthogonality of the orthogonal polynomial. The use of orthogonal collocations can solve the Runge phenomenon [20][21], which were disadvantages of the equally spaced Lagrange interpolation equation. Although N has not been explained here, in the orthogonal collocation finite element method, N represents the number of internal collocations in the element, and in the case of one dimension, two are the boundary condition points (external collocations) at both ends of the element, and the number of local collocations in the element is N + 2 (x_1, x_2, x_3, ..., x_{N+2}) by adding the number of internal collocations N and the number of external collocations 2.

Differential Operators (matrices) with Respect to Space [13][16]

The induction of differential operators in OCFEM is described below, which is a matrix (differential operator) that acts on the solution vector in order to obtain the differential vector of a discrete solution. The method of deriving a differential operator by differentiating the orthogonal polynomial is described below.

On two-dimensional polynomials and differential operators (matrices)

If we assume that the dependent variable u changes only for the independent variables x and y in space, with the time t fixed, then the polynomial of the space two-dimensional is given by the following equation (9).

$$u = \left(\sum_{i=1}^{N_1+2} a_i x^{i-1} \right) \left(\sum_{j=1}^{N_2+2} b_j y^{j-1} \right) = \sum_{i=1}^{N_1+2} \sum_{j=1}^{N_2+2} x^{i-1} y^{j-1} d_{ij} \tag{9}$$

where $d_{ij} = a_i b_j$

Let the p be the number of the local collocation in a element, and (x_p, y_p) is the spatial coordinate value of the collocation p. In the collocation p, u_p is expressed by the following equation (10).

$$u_p = \sum_{i=1}^{N_1+2} \sum_{j=1}^{N_2+2} x_p^{i-1} y_p^{j-1} d_{ij} \tag{10}$$

The following shows the induction of a partial differential operator matrix up to the second order of the two dimensions, and the following equation is obtained by partial differentiating equation (9) to the second order.

$$
\begin{aligned}
\frac{\partial u}{\partial x} &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(i-1)x^{i-2}y^{j-1}d_{ij} \\
\frac{\partial u}{\partial y} &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(j-1)x^{i-1}y^{j-2}d_{ij} \\
\frac{\partial^2 u}{\partial x^2} &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(i-1)(i-2)x^{i-3}y^{j-1}d_{ij} \\
\frac{\partial^2 u}{\partial y^2} &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(j-1)(j-2)x^{i-1}y^{j-3}d_{ij} \\
\frac{\partial^2 u}{\partial x\partial y} &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(i-1)(j-1)x^{i-2}y^{j-2}d_{ij}
\end{aligned}
\tag{11}
$$

The partial derivative at collocation p is as follows (12) from equation (11).

$$
\begin{aligned}
\left.\frac{\partial u}{\partial x}\right|_p &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(i-1)x_p^{i-2}y_p^{j-1}d_{ij} \\
\left.\frac{\partial u}{\partial y}\right|_p &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(j-1)x_p^{i-1}y_p^{j-2}d_{ij} \\
\left.\frac{\partial^2 u}{\partial x^2}\right|_p &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(i-1)(i-2)x_p^{i-3}y_p^{j-1}d_{ij} \\
\left.\frac{\partial^2 u}{\partial y^2}\right|_p &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(j-1)(j-2)x_p^{i-1}y_p^{j-3}d_{ij} \\
\left.\frac{\partial^2 u}{\partial x\partial y}\right|_p &= \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2}(i-1)(j-1)x_p^{i-2}y_p^{j-2}d_{ij}
\end{aligned}
\tag{12}
$$

In order to represent Equation (10) and Equation (12) as vectors and matrices, define vectors and matrices as shown below.

$\mathbf{u} = [u_p]$: Solution vector for collocation p (p=1,2,…,(N_1+2)(N_2+2))

$\mathbf{Q} = [x_p^{i-1}y_p^{j-1}]$: i = 1, 2, …, N_1+2(column), j = 1, 2, …, N_2+2(column), p = 1, 2, …, (N_1+2)(N_2+2)(row), (N_1+2)(N_2+2)×(N_1+2)(N_2+2)matrix

$\mathbf{d} = [d_{ij}]$: Coefficient vector of polynomials, i = 1, 2, …, N_1+2, j = 1, 2, …, N_2+2, (N_1+2)(N_2+2) row vector

$\left[\frac{\partial u}{\partial x}\right] = \left[\left.\frac{\partial u}{\partial x}\right|_p\right]$: Vector of first-order partial derivative with respect to x of u

$\left[\frac{\partial u}{\partial y}\right] = \left[\left.\frac{\partial u}{\partial y}\right|_p\right]$: Vector of first-order partial derivative with respect to y of u

$\left[\frac{\partial^2 u}{\partial x^2}\right] = \left[\left.\frac{\partial^2 u}{\partial x^2}\right|_p\right]$: Vector of second-order partial derivative with respect to x of u

$\left[\frac{\partial^2 u}{\partial y^2}\right] = \left[\left.\frac{\partial^2 u}{\partial y^2}\right|_p\right]$: Vector of second-order partial derivative with respect to y of u

$\left[\frac{\partial^2 u}{\partial x \partial y}\right] = \left[\left.\frac{\partial^2 u}{\partial x \partial y}\right|_p\right]$: Vector of cross-partial derivatives of the second order with respect to x and y of u.

$\mathbf{D_x} = \left[(i-1)x_p^{i-2}y_p^{j-1}\right]$:The numbers i, j, and p are similar to **Q**,$(N_1+2)(N_2+2)\times(N_1+2)(N_2+2)$matrix

$\mathbf{D_y} = \left[(j-1)x_p^{i-1}y_p^{j-2}\right]$: The numbers i, j, and p are similar to **Q**,$(N_1+2)(N_2+2)\times(N_1+2)(N_2+2)$ matrix

$\mathbf{D_{2x}} = \left[(i-1)(i-2)x_p^{i-3}y_p^{j-1}\right]$: The numbers i, j, and p are similar to **Q**, $(N_1+2)(N_2+2)\times(N_1+2)(N_2+2)$matrix

$\mathbf{D_{2y}} = \left[(j-1)(j-2)x_p^{i-1}y_p^{j-3}\right]$: The numbers i, j, and p are similar to **Q**, $(N_1+2)(N_2+2)\times(N_1+2)(N_2+2)$matrix

$\mathbf{D_{2xy}} = \left[(i-1)(j-1)x_p^{i-2}y_p^{j-2}\right]$: The numbers i, j, and p are similar to **Q**, $(N_1+2)(N_2+2)\times(N_1+2)(N_2+2)$matrix

According to the above definitions of vectors and matrices, Equation (10) and Equation (12) are represented as follows equations (13) and (14), respectively.

$$\mathbf{u} = \mathbf{Qd} \tag{13}$$

$$\left[\frac{\partial u}{\partial x}\right] = \mathbf{D_x d} \qquad \left[\frac{\partial u}{\partial y}\right] = \mathbf{D_y d}$$
$$\left[\frac{\partial^2 u}{\partial x^2}\right] = \mathbf{D_{2x} d} \qquad \left[\frac{\partial^2 u}{\partial y^2}\right] = \mathbf{D_{2y} d} \tag{14}$$
$$\left[\frac{\partial^2 u}{\partial x \partial y}\right] = \mathbf{D_{2xy} d}$$

Here, from equation (13)

$$\mathbf{d} = \mathbf{Q}^{-1}\mathbf{u} \tag{15}$$

Therefore, the partial derivative vector of Equation (14) is represented as follows.

$$\left[\frac{\partial u}{\partial x}\right] = \mathbf{D_x d} = \mathbf{D_x Q}^{-1}\mathbf{u} = \mathbf{A_x u}$$
$$\left[\frac{\partial u}{\partial y}\right] = \mathbf{D_y d} = \mathbf{D_y Q}^{-1}\mathbf{u} = \mathbf{A_y u}$$
$$\left[\frac{\partial^2 u}{\partial x^2}\right] = \mathbf{D_{2x} d} = \mathbf{D_{2x} Q}^{-1}\mathbf{u} = \mathbf{B_x u} \tag{16}$$
$$\left[\frac{\partial^2 u}{\partial y^2}\right] = \mathbf{D_{2y} d} = \mathbf{D_{2y} Q}^{-1}\mathbf{u} = \mathbf{B_y u}$$
$$\left[\frac{\partial^2 u}{\partial x \partial y}\right] = \mathbf{D_{2xy} d} = \mathbf{D_{2xy} Q}^{-1} u = \mathbf{C_{xy} u}$$

where $\mathbf{A_x}$ $\mathbf{A_y}$ $\mathbf{B_x}$ $\mathbf{B_y}$ $\mathbf{C_{xy}}$ is a differential operator (matrix), which is expressed by equation (17) below.

$$\mathbf{A_x} = \mathbf{D_x Q}^{-1} \qquad \mathbf{A_y} = \mathbf{D_y Q}^{-1}$$
$$\mathbf{B_x} = \mathbf{D_{2x} Q}^{-1} \qquad \mathbf{B_y} = \mathbf{D_{2y} Q}^{-1} \tag{17}$$
$$\mathbf{C_{xy}} = \mathbf{D_{2xy} Q}^{-1}$$

A differential operator (matrix) has the action of a discrete differential operator, and the differential operator is defined as the following equation (18). [It seems that it is necessary to prove that this is true mathematically]

$$\left[\frac{\partial}{\partial x}\right]=\mathbf{A_x}$$
$$\left[\frac{\partial}{\partial y}\right]=\mathbf{A_y}$$
$$\left[\frac{\partial^2}{\partial x^2}\right]=\mathbf{B_x}=\mathbf{A_x}\mathbf{A_x} \quad (18)$$
$$\left[\frac{\partial^2}{\partial y^2}\right]=\mathbf{B_y}=\mathbf{A_y}\mathbf{A_y}$$
$$\left[\frac{\partial^2}{\partial x \partial y}\right]=\mathbf{C_{xy}}=\mathbf{A_x}\mathbf{A_y}=\mathbf{A_y}\mathbf{A_x}$$

It has been numerically verified that even if the order of the derivatives is reshuffled in cross-partial derivatives, they are equal and commutative. When the differential operator (matrix) defined by equation (18) is applied to the solution vector, each partial derivative vector is obtained. When calculated numerically by Equation (17), the inverse matrix is included, so when the order (internal collocation order N1, N2) increases, a differential operator (matrix) with poor accuracy is calculated. It can be seen that the differential operator (matrix) is the same as the coefficient matrix (collocation constant) derived using the two-dimensional Lagrange interpolation formula. In the next section, we show that differential operators are represented and computed using the two-dimensional Lagrange interpolation formula.

Calculation method using the Lagrange interpolation formula for differential operators (matrices) [19][4]

The two-dimensional polynomial is expressed by the Lagrange interpolation formula, as shown in Equation (19), where the position of the collocation is (x_i, y_j) as the root of the Sifted Legendre polynomial. The range of the Sifted Legendre polynomial is (0,1), and the range of the Legendre polynomial (-1,1) is converted to (0,1).

$$u(x,y)=\sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2} l_i(x)\, l_j(y)\, u(x_i, y_j) \quad (19)$$

where

$$l_i(x)=\prod_{\substack{k=1\\k\neq i}}^{N_1+2}\frac{x-x_k}{x_i-x_k} \qquad l_j(y)=\prod_{\substack{k=1\\k\neq j}}^{N_2+2}\frac{y-y_k}{y_j-y_k} \quad (20)$$

The above equation (19) is partial differentiated by x and y, and the partial derivative at the collocations m (number in the x direction) and n (number in the y direction) is shown below.

$$\left.\frac{\partial u}{\partial x}\right|_{m,n} = \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2} l_i'\left(x_m\right) l_j\left(y_n\right) u\left(x_i, y_j\right)$$
$$\left.\frac{\partial u}{\partial y}\right|_{m,n} = \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2} l_i\left(x_m\right) l_j'\left(y_n\right) u\left(x_i, y_j\right)$$
$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{m,n} = \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2} l_i''\left(x_m\right) l_j\left(y_n\right) u\left(x_i, y_j\right) \tag{21}$$
$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{m,n} = \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2} l_i\left(x_m\right) l_j''\left(y_n\right) u\left(x_i, y_j\right)$$
$$\left.\frac{\partial^2 u}{\partial x \partial y}\right|_{m,n} = \sum_{i=1}^{N_1+2}\sum_{j=1}^{N_2+2} l_i'\left(x_m\right) l_j'\left(y_n\right) u\left(x_i, y_j\right)$$

From equation (21), the differential operator (matrix) is represented by equation (22), where (′) and (") are first-order derivatives and second-order derivatives respectively.

$$\begin{aligned}
\mathbf{A_x} &= l_i'(x_m) l_j(y_n) \\
\mathbf{A_y} &= l_i(x_m) l_j'(y_n) \\
\mathbf{B_x} &= l_i''(x_m) l_j(y_n) \\
\mathbf{B_y} &= l_i(x_m) l_j''(y_n) \\
\mathbf{C_{xy}} &= l_i'(x_m) l_j'(y_n)
\end{aligned} \tag{22}$$

Differential Operators (Matrices) with Respect to Time (13)(14)

If we fix it in space q and express the dependent variable u in space q with a polynomial with respect to time, we get Equation (23).

$$u^q = \sum_{j=1}^{N_t+1} b_j^q t^{j-1} \tag{23}$$

u^q : The value of the dependent variable for the change in time when the spatial collocation q is fixed.

b_j^q : Coefficients of the polynomial with respect to time when the spatial collocation q is fixed.

The first-order derivative of equation (23) with respect to t yields Equation (24).

$$\frac{\partial u^q}{\partial t} = \sum_{j=1}^{N_t+1} (j-1) t^{j-2} b_j^q \tag{24}$$

u_i^q and first order derivative with respect to t at time collocation i are as follow equation.

$$u_i^q = \sum_{j=1}^{N_t+1} b_j^q t_i^{j-1}$$
$$\left.\frac{\partial u^q}{\partial t}\right|_i = \sum_{j=1}^{N_t+1} \left(j-1\right) t_i^{j-2} b_j^q \tag{25}$$

representation by vector and matrix are as follow

$$\mathbf{u}^q = \mathbf{Q}\mathbf{b}^q \qquad \mathbf{Q} = \left[t_i^{j-1}\right]$$
$$\left[\frac{\partial u^q}{\partial t}\right] = \mathbf{D}\mathbf{b}^q \qquad \mathbf{D} = \left[\left(j-1\right) t_i^{j-2}\right] \tag{26}$$

First order derivative with respect to t of u is as follow

$$\left[\frac{\partial u^q}{\partial t}\right] = \mathbf{D}\mathbf{b}^q = \mathbf{D}\mathbf{Q}^{-1}\mathbf{u}^q = \mathbf{A_t}\mathbf{u}^q \tag{27}$$

it can be seen from the basic concept of partial derivatives that the differential operators (matrices) of the first order are derived by the same way of thinking as space, but this differential operator (matrix) with respect to time does not depend on the space q.

Since the differential operator (matrix) of time can be created using the same concept as the differential operator (matrix) of one-dimensional space, it can be obtained by differentiating the one-dimensional Lagrange interpolation formula with orthogonal collocations.

Coordinate Transformation Matrix Required for Unstructured Grids(12)(14)~(16)(22)

In the Galerkin method, which is one of the weighted residual methods, it is expressed in the form of an integral, and the conversion to an unstructured grid is possible by using Jacobian. However, in the OCFEM (Orthogonal Collocation Finite Element Method), the partial derivative at the discrete collocations (orthogonal collocations) in the element must be converted from the local coordinate system to the global coordinate system (unstructured grids), which can be achieved by using the concept of partial derivative of the composite function. This transformation must be performed for a total of five partial derivatives (including cross-partial derivatives) for the dependent variable u, two for first-order partial derivatives (ξ, η) and three for second-order partial derivatives (ξ, η). The reason why it is not necessary to convert the higher-order partial derivatives of 3 or more orders is that it is necessary to convert the PDEs of the higher order to the PDEs of the second order or less. It has been shown that this makes it easier to set boundary conditions.

Define the coordinate transformation function used for the composite function for converting the local coordinate system to the global coordinate system (unstructured grid) as shown in Equation (28).

$$\begin{aligned} x &= g(\xi,\eta) \\ y &= h(\xi,\eta) \end{aligned} \tag{28}$$

If the dependent variable is u, the partial derivative of the composite function is calculated as shown in Equation (29).

$$\begin{aligned} \frac{\partial u}{\partial \xi} &= \frac{\partial u}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \xi} \\ \frac{\partial u}{\partial \eta} &= \frac{\partial u}{\partial x}\frac{\partial x}{\partial \eta} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \eta} \end{aligned} \tag{29}$$

The partial derivative of the second order can be derived as follows.

$$\begin{aligned} \frac{\partial^2 u}{\partial \xi^2} &= \frac{\partial}{\partial \xi}\left(\frac{\partial u}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \xi}\right) = \frac{\partial^2 u}{\partial x^2}\left(\frac{\partial x}{\partial \xi}\right)^2 + \frac{\partial^2 u}{\partial x \partial y}\frac{\partial y}{\partial \xi}\frac{\partial x}{\partial \xi} + \frac{\partial^2 u}{\partial y \partial x}\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \xi} + \frac{\partial^2 u}{\partial y^2}\left(\frac{\partial y}{\partial \xi}\right)^2 + \frac{\partial u}{\partial x}\frac{\partial^2 x}{\partial \xi^2} + \frac{\partial u}{\partial y}\frac{\partial^2 y}{\partial \xi^2} \\ &= \frac{\partial^2 u}{\partial x^2}\left(\frac{\partial x}{\partial \xi}\right)^2 + 2\frac{\partial^2 u}{\partial x \partial y}\left(\frac{\partial x}{\partial \xi}\right)\left(\frac{\partial y}{\partial \xi}\right) + \frac{\partial^2 u}{\partial y^2}\left(\frac{\partial y}{\partial \xi}\right)^2 + \frac{\partial u}{\partial x}\frac{\partial^2 x}{\partial \xi^2} + \frac{\partial u}{\partial y}\frac{\partial^2 y}{\partial \xi^2} \end{aligned} \tag{30}$$

$$\begin{aligned} \frac{\partial^2 u}{\partial \eta^2} &= \frac{\partial}{\partial \eta}\left(\frac{\partial u}{\partial x}\frac{\partial x}{\partial \eta} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \eta}\right) = \frac{\partial^2 u}{\partial x^2}\left(\frac{\partial x}{\partial \eta}\right)^2 + \frac{\partial^2 u}{\partial x \partial y}\frac{\partial y}{\partial \eta}\frac{\partial x}{\partial \eta} + \frac{\partial^2 u}{\partial y \partial x}\frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \eta} + \frac{\partial^2 u}{\partial y^2}\left(\frac{\partial y}{\partial \eta}\right)^2 + \frac{\partial u}{\partial x}\frac{\partial^2 x}{\partial \eta^2} + \frac{\partial u}{\partial y}\frac{\partial^2 y}{\partial \eta^2} \\ &= \frac{\partial^2 u}{\partial x^2}\left(\frac{\partial x}{\partial \eta}\right)^2 + 2\frac{\partial^2 u}{\partial y \partial x}\left(\frac{\partial x}{\partial \eta}\right)\left(\frac{\partial y}{\partial \eta}\right) + \frac{\partial^2 u}{\partial y^2}\left(\frac{\partial y}{\partial \eta}\right)^2 + \frac{\partial u}{\partial x}\frac{\partial^2 x}{\partial \eta^2} + \frac{\partial u}{\partial y}\frac{\partial^2 y}{\partial \eta^2} \end{aligned} \tag{31}$$

$$\begin{aligned} \frac{\partial^2 u}{\partial \xi \partial \eta} &= \frac{\partial}{\partial \eta}\left(\frac{\partial u}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \xi}\right) = \frac{\partial^2 u}{\partial x^2}\frac{\partial x}{\partial \eta}\frac{\partial x}{\partial \xi} + \frac{\partial^2 u}{\partial x \partial y}\frac{\partial y}{\partial \eta}\frac{\partial x}{\partial \xi} + \frac{\partial^2 u}{\partial y \partial x}\frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi} + \frac{\partial^2 u}{\partial y^2}\frac{\partial y}{\partial \eta}\frac{\partial y}{\partial \xi} + \frac{\partial u}{\partial x}\frac{\partial^2 x}{\partial \xi \partial \eta} + \frac{\partial u}{\partial y}\frac{\partial^2 y}{\partial \xi \partial \eta} \\ &= \frac{\partial^2 u}{\partial x^2}\left(\frac{\partial x}{\partial \xi}\right)\left(\frac{\partial x}{\partial \eta}\right) + \frac{\partial^2 u}{\partial x \partial y}\left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}\right) + \frac{\partial^2 u}{\partial y^2}\left(\frac{\partial y}{\partial \xi}\right)\left(\frac{\partial y}{\partial \eta}\right) + \frac{\partial u}{\partial x}\frac{\partial^2 x}{\partial \xi \partial \eta} + \frac{\partial u}{\partial y}\frac{\partial^2 y}{\partial \xi \partial \eta} \end{aligned} \tag{32}$$

When the above equation group (29) ~ (32) is represented as a matrix, it becomes as Equation (33).

$$\begin{bmatrix} \frac{\partial u}{\partial \xi} \\ \frac{\partial u}{\partial \eta} \\ \frac{\partial^2 u}{\partial \xi^2} \\ \frac{\partial^2 u}{\partial \eta^2} \\ \frac{\partial^2 u}{\partial \xi \partial \eta} \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & 0 & 0 & 0 \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & 0 & 0 & 0 \\ \frac{\partial^2 x}{\partial \xi^2} & \frac{\partial^2 y}{\partial \xi^2} & \left(\frac{\partial x}{\partial \xi}\right)^2 & \left(\frac{\partial y}{\partial \xi}\right)^2 & 2\left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \xi}\right) \\ \frac{\partial^2 x}{\partial \eta^2} & \frac{\partial^2 y}{\partial \eta^2} & \left(\frac{\partial x}{\partial \eta}\right)^2 & \left(\frac{\partial y}{\partial \eta}\right)^2 & 2\left(\frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \eta}\right) \\ \frac{\partial^2 x}{\partial \xi \partial \eta} & \frac{\partial^2 y}{\partial \xi \partial \eta} & \left(\frac{\partial x}{\partial \xi}\right)\left(\frac{\partial x}{\partial \eta}\right) & \left(\frac{\partial y}{\partial \xi}\right)\left(\frac{\partial y}{\partial \eta}\right) & \left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} + \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}\right) \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \\ \frac{\partial^2 u}{\partial x^2} \\ \frac{\partial^2 u}{\partial y^2} \\ \frac{\partial^2 u}{\partial x \partial y} \end{bmatrix} \tag{33}$$

$$\mathbf{T}=\begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & 0 & 0 & 0 \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & 0 & 0 & 0 \\ \frac{\partial^2 x}{\partial \xi^2} & \frac{\partial^2 y}{\partial \xi^2} & \left(\frac{\partial x}{\partial \xi}\right)^2 & \left(\frac{\partial y}{\partial \xi}\right)^2 & 2\left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \xi}\right) \\ \frac{\partial^2 x}{\partial \eta^2} & \frac{\partial^2 y}{\partial \eta^2} & \left(\frac{\partial x}{\partial \eta}\right)^2 & \left(\frac{\partial y}{\partial \eta}\right)^2 & 2\left(\frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \eta}\right) \\ \frac{\partial^2 x}{\partial \xi \partial \eta} & \frac{\partial^2 y}{\partial \xi \partial \eta} & \left(\frac{\partial x}{\partial \xi}\right)\left(\frac{\partial x}{\partial \eta}\right) & \left(\frac{\partial y}{\partial \xi}\right)\left(\frac{\partial y}{\partial \eta}\right) & \left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta}+\frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}\right) \end{bmatrix} \tag{34}$$

and if the inverse matrix is $\mathbf{J}=\mathbf{T}^{-1}$, differential vector of u is represented equation (35) as follow

$$\begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \\ \frac{\partial^2 u}{\partial x^2} \\ \frac{\partial^2 u}{\partial y^2} \\ \frac{\partial^2 u}{\partial x \partial y} \end{bmatrix} = \mathbf{J} \begin{bmatrix} \frac{\partial u}{\partial \xi} \\ \frac{\partial u}{\partial \eta} \\ \frac{\partial^2 u}{\partial \xi^2} \\ \frac{\partial^2 u}{\partial \eta^2} \\ \frac{\partial^2 u}{\partial \xi \partial \eta} \end{bmatrix} \tag{35}$$

J represents the transformation of partial derivatives in local coordinates to partial derivatives in the global coordinate system, and this **J** is named the coordinate transformation matrix. Eliminating u from Equation (35), we consider the transformation of the differential operator from the local coordinates to the global coordinate system, and it is expressed as Equation (36).

$$\begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial^2}{\partial x^2} \\ \frac{\partial^2}{\partial y^2} \\ \frac{\partial^2}{\partial x \partial y} \end{bmatrix} = \mathbf{J} \begin{bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial^2}{\partial \xi^2} \\ \frac{\partial^2}{\partial \eta^2} \\ \frac{\partial^2}{\partial \xi \partial \eta} \end{bmatrix} \tag{36}$$

$$\begin{aligned} \mathbf{A}_{\xi} &= \left[\frac{\partial}{\partial \xi}\right] & \mathbf{A}_{x} &= \left[\frac{\partial}{\partial x}\right] \\ \mathbf{A}_{\eta} &= \left[\frac{\partial}{\partial \eta}\right] & \mathbf{A}_{y} &= \left[\frac{\partial}{\partial y}\right] \\ \mathbf{B}_{\xi} &= \left[\frac{\partial^2}{\partial \xi^2}\right] & \mathbf{B}_{x} &= \left[\frac{\partial^2}{\partial x^2}\right] \\ \mathbf{B}_{\eta} &= \left[\frac{\partial^2}{\partial \eta^2}\right] & \mathbf{B}_{y} &= \left[\frac{\partial^2}{\partial y^2}\right] \\ \mathbf{C}_{\xi\eta} &= \left[\frac{\partial^2}{\partial \xi \partial \eta}\right] & \mathbf{C}_{xy} &= \left[\frac{\partial^2}{\partial x \partial y}\right] \end{aligned} \tag{37}$$

If the elements of **J** are J_{ij} (i=1,2,3,4,5 j=1,2,3,4,5), the following equations (38) are obtained from equations (36) and (37).

$$\begin{aligned}
\mathbf{A_x} &= J_{11}\mathbf{A}_\xi + J_{12}\mathbf{A_\eta} + J_{13}\mathbf{B}_\xi + J_{14}\mathbf{B_\eta} + J_{15}\mathbf{C_{\xi\eta}} \\
\mathbf{A_y} &= J_{21}\mathbf{A}_\xi + J_{22}\mathbf{A_\eta} + J_{23}\mathbf{B}_\xi + J_{24}\mathbf{B_\eta} + J_{25}\mathbf{C_{\xi\eta}} \\
\mathbf{B_x} &= J_{31}\mathbf{A}_\xi + J_{32}\mathbf{A_\eta} + J_{33}\mathbf{B}_\xi + J_{34}\mathbf{B_\eta} + J_{35}\mathbf{C_{\xi\eta}} \\
\mathbf{B_y} &= J_{41}\mathbf{A}_\xi + J_{42}\mathbf{A_\eta} + J_{43}\mathbf{B}_\xi + J_{44}\mathbf{B_\eta} + J_{45}\mathbf{C_{\xi\eta}} \\
\mathbf{C_{xy}} &= J_{51}\mathbf{A}_\xi + J_{52}\mathbf{A_\eta} + J_{53}\mathbf{B}_\xi + J_{54}\mathbf{B_\eta} + J_{55}\mathbf{C_{\xi\eta}}
\end{aligned} \tag{38}$$

The following relationship that was established in the local coordinate system (ξ, η)

$$\begin{aligned}
&\mathbf{B_x} = \mathbf{A_x}\mathbf{A_x}, \quad \mathbf{B_y} = \mathbf{A_y}\mathbf{A_y}, \\
&\mathbf{C_{xy}} = \mathbf{A_x}\mathbf{A_y} = \mathbf{A_y}\mathbf{A_x}
\end{aligned} \tag{39}$$

is not true. (in numerical calculation)

The coordinate transformation function is as follow specifically for quadrilateral elements.

$$\begin{aligned}
x &= a_1 + a_2\xi + a_3\eta + a_4\xi\eta \\
y &= b_1 + b_2\xi + b_3\eta + b_4\xi\eta
\end{aligned} \tag{40}$$

$$\begin{aligned}
&\frac{\partial x}{\partial \xi} = a_2 + a_4\eta \qquad \frac{\partial y}{\partial \xi} = b_2 + b_4\eta \\
&\frac{\partial x}{\partial \eta} = a_3 + a_4\xi \qquad \frac{\partial y}{\partial \eta} = b_3 + b_4\xi \\
&\frac{\partial^2 x}{\partial \xi^2} = 0 \qquad \frac{\partial^2 y}{\partial \xi^2} = 0 \\
&\frac{\partial^2 x}{\partial \eta^2} = 0 \qquad \frac{\partial^2 y}{\partial \eta^2} = 0 \\
&\frac{\partial^2 x}{\partial \xi \partial \eta} = a_4 \qquad \frac{\partial^2 y}{\partial \xi \partial \eta} = b_4
\end{aligned} \tag{41}$$

For a_1, a_2, a_3, a_4, b_1, b_2, b_3, b_4, equations can be derived (calculated) by correlating the four corners of the global coordinate system (x, y) [(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4)] to the four corner points of the local coordinates (ξ, η)[(0, 0), (1, 0), (1, 1), (1, 1), (0, 1)]. Using these a_1, a_2, a_3, a_4, b_1, b_2, b_3, and b_4, the partial derivative values for the coordinates of Equation (40) are calculated, and the coordinate transformation matrix **J** is specifically calculated.

First, fix the rows of the partial differential operator matrix, for example, if you fix the *i* rows, the matrix **T** is calculated for the *i* collocations (ξ_i, η_i) because we are focusing on the *i*-collocations. **J** is calculated using the inverse matrix of the matrix **T** with respect to the i-collocation, and from equation (38), the i row of the partial differential operator matrix of the global coordinate system (i collocation) is calculated.

Local Numbering within an Element (13)(16)

As a simple example, in order to represent the orthogonal collocations using the roots of the orthogonal polynomial in the x-direction of the Nth order and the roots of the orthogonal polynomials in the y-direction of the Nth order, the numbers of the roots in the x- and y-directions are i=2~N+1 and j=2~N+1 as internal collocations. i = 1 and N+2, j = 1 and N + 2 are boundary points (element boundary points (nodes collocations (side collocations), node collocations (4 corner collocations)): external collocations) (Fig. 1). Here, N is the number of internal collocations in the x and y directions, and N = N1 = N2 for simplicity. Similar to (i, j), (m, n) have the same numbering.

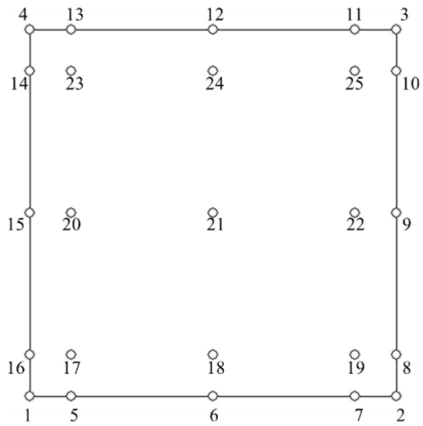


Fig.1 allocation of collocation in a element

If N = 3 (Fig.1)

Internal collocation, 3×3 (N×N)

Node collocations (4 corner collocations) (external collocation), 4

Nodes collocations(side collocations)(external collocation) 4×3 (4×N)

Total collocations: $5\times5=25$ $4+4\times N+N\times N=(N+2)(N+2)$

(i, j) corresponds to the local collocation number p=1～(N+2)(N+2), and the collocation position is ordered as follows. (1~25 in the example in the figure 1)

p=1～4 Node collocations (4 corner collocations) (external collocation)

p=5～4+4N Nodes collocations(side collocations)(external collocation)

p=5+4N～(N+2)(N+2)internal collocation

external collocation :r =1～4+4N（4 corner collocations:1～4）

internal collocation :q =5+4N～(N+2)(N+2)

(Total collocation＝external collocation＋internal collocation)

The global collocation number T is represented by the element k and the local collocation number p by the following relation.

$$T = IE(p,k) \tag{42}$$

Here, IE is a function that relates p, k and T. (where k is the element number)

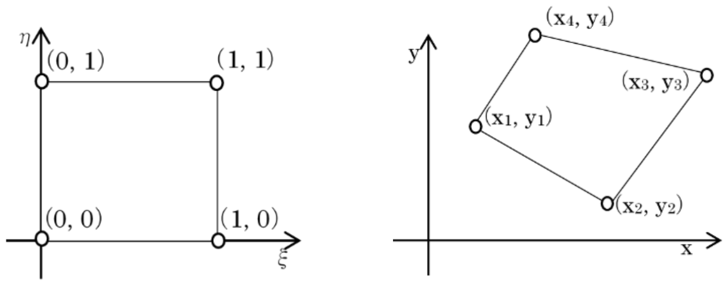
Thus, if the numbering (i, j), (m, n) in the x and y directions corresponds to the local collocation number p in the element, the differential operator (matrix) becomes a square matrix of (N+2) (N+2) ×(N+2) (N+2). This differential operator (matrix) is not regular, and when formulating the basic equation and the boundary condition equation, the differential operator (matrix $\mathbf{A}_{\mathbf{x}qp}$) of the internal collocation q is used in the basic equation (established by the internal collocation), and the differential operator (matrix $\mathbf{A}_{\mathbf{x}rp}$) of the external collocation r is used in the element boundary condition expressed by partial derivatives. The number of all points for the element is p = q + r, where q is the number of internal points and r is the number of external points (number of element boundary points). If the differential operator matrix is divided into a matrix of qp (not a square matrix: an internal collocation differential operator matrix $\mathbf{A}_{\mathbf{x}qp}$) and a matrix of rp (not a square matrix: an external collocation differential operator matrix $\mathbf{A}_{\mathbf{x}rp}$) , the PDE's is formulated by the basic equation (internal collocation) and the boundary condition equation (external collocation) using the differential operator, and by superposition (element connection), it becomes an overall regular square matrix, which results in solving a system of equations.

Gauss numerical integration in OCFEM (4)(15)(22)

Area integration of the quadrilateral element

As a specific example, the preparation for calculating the total substrate consumption rate in a biofilm region (Biofilm) by the Gauss integral formula is shown below. The relationship between the global coordinates (x, y) and the local coordinates (ξ, η) is expressed by the following equation (43).

$$x=\phi(\xi,\eta),\quad y=\psi(\xi,\eta) \tag{43}$$



Local coordinate system　　　Global coordinate system
(no representation of orthogonal collocation)

Fig.2 Local coordinate system and Global coordinate system in case of quadrilateral element

In the case of the quadrilateral element shown in Fig.2, the conversion formula from the local coordinate system to the quadrilateral element of the global coordinate system is expressed by Equation (44).

$$\begin{aligned} x &= a_1 + a_2\xi + a_3\eta + a_4\xi\eta \\ y &= b_1 + b_2\xi + b_3\eta + b_4\xi\eta \end{aligned} \tag{44}$$

The coefficients a_i and b_i are obtained from the correspondence between the four corners of the rectangular element, which is the local coordinate, and the four corners of the quadrilateral element, which is the global coordinate (Fig. 2).

$$\begin{aligned} a_1 &= x_1 \\ b_1 &= y_1 \\ a_2 &= x_2 - x_1 \\ b_2 &= y_2 - y_1 \\ a_3 &= x_4 - x_1 \\ b_3 &= y_4 - y_1 \\ a_4 &= (x_1 + x_3) - (x_2 + x_4) \\ b_4 &= (y_1 + y_3) - (y_2 + y_4) \end{aligned} \tag{45}$$

In the $x-y$ coordinate system, let the integrable function be $f(x, y)$. In the $\xi-\eta$ coordinate system, it is expressed as follows.

$$f(x, y) = f\left(\varphi(\xi, \eta), \psi(\xi, \eta)\right) \tag{46}$$

Here, Jacobian for integrating conversion from a $x-y$ coordinate system to a $\xi-\eta$ coordinate system in a certain integral region is expressed by the following equation.

$$\begin{aligned}\left|J(\xi,\eta)\right| &= \left|\frac{D(x,y)}{D(\xi,\eta)}\right| = \begin{vmatrix}\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}\end{vmatrix} = \frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi} \\ &= \left(a_2 + a_4\eta\right)\left(b_3 + b_4\xi\right) - \left(a_3 + a_4\xi\right)\left(b_2 + b_4\eta\right)\end{aligned} \tag{47}$$

Therefore, the integral is expressed by Equation (48).

$$\iint_A f(x, y)dxdy = \iint_B f\left(\varphi(\xi,\eta),\psi(\xi,\eta)\right)\left|J(\xi,\eta)\right|d\xi d\eta \tag{48}$$

where A is the area of quadrilateral elements in the global coordinate system, and B is the region of rectangular elements in the local coordinate system. Here, since $f(\varphi(\xi, \eta), \psi(\xi, \eta))$ has already been calculated by the orthogonal point finite element method (OCFEM), it is possible to calculate the integral using the weights in the $\xi-\eta$ coordinate system. Note that the orthogonal collocation of the Legendre polynomial in OCFEM and the integration point of Gauss's integral formula are the same.

Specifically, the discrete representation is as following equation (49). Since the integrating point is the internal collocation of the element, the weight of $i = 5 + 4.\ N\sim(N+2)(N+2)$ and the Jacobian use give the discretized integral formula (49), where the total number of elements in the global coordinate system is m.

$$\begin{aligned}&\iint_A f(x,y)\,dxdy = \iint_B f\left(\phi(\xi,\eta),\psi(\xi,\eta)\right)\left|J(\xi,\eta)\right|d\xi d\eta \\ &\approx \sum_{j=1}^{m}\sum_{i=5+4\cdot N}^{(N+2)(N+2)} f^{j}\left(\phi(\xi_i,\eta_i),\psi(\xi_i,\eta_i)\right)W_i\left(\left(a_2+a_4\eta_i\right)\left(b_3+b_4\xi_i\right)-\left(a_3+a_4\xi_i\right)\left(b_2+b_4\eta_i\right)\right)\end{aligned} \tag{49}$$

$(k = 1\sim N)$: number of internal collocation in ξ direction

$(l = 1\sim N)$: number of internal collocation in η direction

$\left(i = 4 + 4N + l + N(k-1)\right)$

$$W_i = W_{1l}W_{1k} \tag{50}$$

W_{1l}, W_{1k} is weight in the one-dimensional direction,

W_i is weight in the two-dimensional direction.

Line integrals on the boundary edges of quadrilateral elements

In order to specifically calculate the flux flowing into and out of the biofilm surface, it is necessary to prepare a line integral that calculates the total flux on the edge corresponding to the surface portion of the quadrilateral element on the biofilm surface.

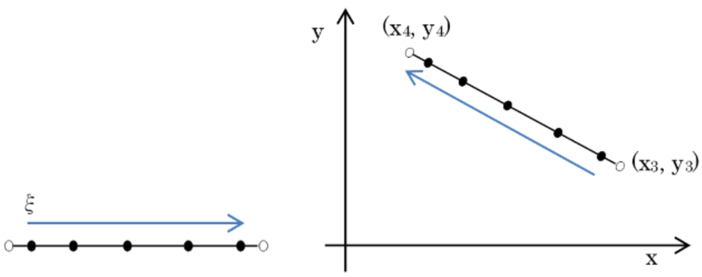


Fig.3 Local coordinate system and global coordinate system in a side of quadrilateral element

As shown in Fig.3, the edges (x, y) of the global coordinate system are represented by the sides (ξ) of the local coordinate system.

$$\begin{aligned} x &= a_1 + a_2\xi = \varphi(\xi) \\ y &= b_1 + b_2\xi = \psi(\xi) \end{aligned} \qquad (51)$$

$$\left.\begin{aligned} &when\ \xi = 0,\ (x, y) = (x_3, y_3) \\ &when\ \xi = 1,\ (x, y) = (x_4, y_4) \end{aligned}\right\} \qquad (52)$$

From the relationship of the above equation

$$\begin{aligned} &x_3 = a_1 && a_1 = x_3 \\ &y_3 = b_1 && b_1 = y_3 \\ &x_4 = a_1 + a_2 && a_2 = x_4 - a_1 = x_4 - x_3 \\ &y_4 = b_1 + b_2 && b_2 = y_4 - b_1 = y_4 - y_3 \end{aligned} \qquad (53)$$

Line integration of $f(x, y)$ is represented by as following equation.

$$\int_L f(x, y)\,ds = \int_l f(\varphi(\xi), \psi(\xi))\sqrt{\left(\frac{dx}{d\xi}\right)^2 + \left(\frac{dy}{d\xi}\right)^2}\,d\xi \qquad (54)$$

Specifically, the line integration at the sides of the global coordinate system is shown as follows.

$$\int_L f(x,y)\,ds = \int_l f(x,y)\sqrt{a_2^2+b_2^2}\,d\xi \tag{55}$$

Representation of discrete Gauss integration is as following equation.

$$\begin{aligned}\int_l f(x,y)\sqrt{a_2^2+b_2^2}\,d\xi &\approx \sum_{i=1}^{NA} W_i f(x_i,y_i)\sqrt{a_2^2+b_2^2} \\ &= \sum_{i=1}^{NA} W_i f\left(\varphi(\xi_i),\psi(\xi_i)\right)\sqrt{a_2^2+b_2^2}\end{aligned} \tag{56}$$

W_i : Weights at the integration point i of the Gauss integral formula

Formulation and Numerical Calculation of Biofilm Model by Differential Operator of Time and Space in Orthogonal Collocation Finite Elements Method

The three main tools of OCFEM are differential operators of matrix representation in space and time, coordinate transformation matrices for unstructured grids, and numerical integration using Gauss integration points that are the same as Legendre's orthogonal collocations. In this paper, we present an example of numerical analysis using OCFEM of an advection-diffusion-reaction equation with a nonlinear reaction term, which is a two-substrate limit biofilm model in two regions (biofilm region and diffusion layer region) (4)(12)(15)(22). Problems in these two domains with different partial differential equations suggest the application of OCFEM to coupled problems such as fluid-structure systems. In this paper, we use a biofilm model as an example, but the main purpose is to expand the application of OCFEM to partial differential equations (PDEs) in science and engineering.

Biofilm model on membrane

Regarding the problem of OCFEM accuracy (comparison with exact numerical solutions), we will leave it to the literature (12)(14) dealing with Laplace equations and heat conduction equations, and here, we will focus on the biofilm model described by the advection-diffusion reaction equation, and the concentration distribution (OCFEM), substrate consumption rate (area within the element), and flux on the biofilm surface (line integration of the element edges) are discussed. The basic equations and boundary conditions for the biofilm region described by the advection-diffusion reaction equation of the two-substrate limit and the diffusion layer region described by the advection-diffusion equation in which microorganisms are absent are shown below.

Biofilm domain：

$$\frac{\partial S}{\partial t}+u\frac{\partial S}{\partial x}+v\frac{\partial S}{\partial y}-D_{sf}\frac{\partial^2 S}{\partial x^2}-D_{sf}\frac{\partial^2 S}{\partial y^2}-f(S,C)=0$$
$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}-D_{cf}\frac{\partial^2 C}{\partial x^2}-D_{cf}\frac{\partial^2 C}{\partial y^2}-\alpha f(S,C)=0 \quad (57)$$

Diffusion layer domain：

$$\frac{\partial S}{\partial t}+u\frac{\partial S}{\partial x}+v\frac{\partial S}{\partial y}-D_{s}\frac{\partial^2 S}{\partial x^2}-D_{s}\frac{\partial^2 S}{\partial y^2}=0$$
$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}-D_{cf}\frac{\partial^2 C}{\partial x^2}-D_{cf}\frac{\partial^2 C}{\partial y^2}=0 \quad (58)$$

where specific substrate consumption rate is represented by following equation (24)

$$f(S,C)=\frac{\upsilon_{\max}S}{K_s+S}\frac{C}{K_c+C} \quad (59)$$

The α is the stoichiometric ratio of substrate S and oxygen C.

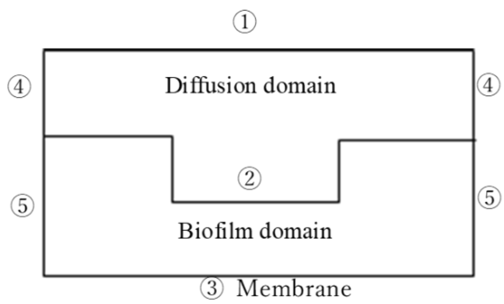


Fig.3 Boundary condition in example domain

The schematic diagram of the boundary condition is shown in Fig.3, and the boundary condition equation is shown in ①~ ⑤, The same is true for *C*.

① $S=S_0 \quad C=C_0$

② Boundary between biofilm and diffusion layer

$$\left(uS-D_{sf}\frac{\partial S}{\partial x}\right)l+\left(vS-D_{sf}\frac{\partial S}{\partial y}\right)m=\left(uS-D_{s}\frac{\partial S}{\partial x}\right)l+\left(vS-D_{s}\frac{\partial S}{\partial y}\right)m \quad (60)$$

③ on membrane：

$$D_{sf}\frac{\partial S}{\partial x}l+D_{sf}\frac{\partial S}{\partial y}m=0 \quad (61)$$

④ $$\left(uS - D_s \frac{\partial S}{\partial x}\right)l + \left(uS - D_s \frac{\partial S}{\partial y}\right)m = 0 \tag{62}$$

⑤ $$\left(uS - D_{sf} \frac{\partial S}{\partial x}\right)l + \left(uS - D_{sf} \frac{\partial S}{\partial y}\right)m = 0 \tag{63}$$

Initial condition：

$$S = \frac{S_0}{2} \qquad C = \frac{C_0}{2} \quad (t = 0) \tag{64}$$

Element boundary condition(Element connection condition)：

$$\begin{aligned} \left\{\left(uS - D_{sf} \frac{\partial S}{\partial x}\right)l + \left(vS - D_{sf} \frac{\partial S}{\partial y}\right)m\right\}^{e1} &= \left\{\left(uS - D_{sf} \frac{\partial S}{\partial x}\right)l + \left(vS - D_{sf} \frac{\partial S}{\partial y}\right)m\right\}^{e2} \\ \left\{\left(uC - D_{cf} \frac{\partial C}{\partial x}\right)l + \left(vC - D_{cf} \frac{\partial C}{\partial y}\right)m\right\}^{e1} &= \left\{\left(uC - D_{cf} \frac{\partial C}{\partial x}\right)l + \left(vC - D_{cf} \frac{\partial C}{\partial y}\right)m\right\}^{e2} \end{aligned} \tag{65}$$

where,

S: Substrate(glucose) concentration[mg/l]

C: Oxygen concentration[mg/l]

u,v: Advective velocity[cm/s]

D_{sf}: Diffusivity of substrate within Biofilm [cm^2/s]

D_{cf}: Diffusivity of oxygen within Biofilm[cm^2/s]

D_s: Diffusivity of substrate in water[cm^2/s]

D_c: Diffusivity of oxygen in water[cm^2/s]

x,y: Position within Biofilm or Diffusion layer[cm]

t: Time[s]

$f(S,C)$: Specific substrate consumption rate[1/s]

v_{max}: Maximum specific substrate consumption rate[1/s]

K_S: Saturation coefficient for substrate[mg/l]

K_C: Saturation coefficient for oxygen[mg/l]

α: Stoichiometric ratio between substrate(S) and oxygen(C)

Formulation of Biofilm model by differential operator in space and time

Here, the formulation by OCFEM in the biofilm and diffusion layer at the internal collocation of an element is shown. The partial derivative of space and time is expressed as a differential operator (matrix) as follows. q is the internal collocation, p is the total collocation (external collocation r and internal collocation q), and i and s are time collocations.

Internal collocation：Biofilm

$$\begin{aligned}&\mathbf{A}_{\mathbf{t}is}\mathbf{S}_{qs}+u_{qi}\mathbf{A}_{\mathbf{x}qp}\mathbf{S}_{pi}+v_{qi}\mathbf{A}_{\mathbf{y}qp}\mathbf{S}_{pi}-D_{sf}\mathbf{B}_{\mathbf{x}qp}\mathbf{S}_{pi}-D_{sf}\mathbf{B}_{\mathbf{y}qp}\mathbf{S}_{pi}-f(S_{qi},C_{qi})=0\\&\mathbf{A}_{\mathbf{t}is}C_{qs}+u_{qi}\mathbf{A}_{\mathbf{x}qp}\mathbf{C}_{pi}+v_{qi}\mathbf{A}_{\mathbf{y}qp}\mathbf{C}_{pi}-D_{cf}\mathbf{B}_{\mathbf{x}qp}\mathbf{C}_{pi}-D_{cf}\mathbf{B}_{\mathbf{y}qp}\mathbf{C}_{pi}-\alpha f(S_{qi},C_{qi})=0\end{aligned}\tag{66}$$

Internal collocation：Diffusion layer

$$\begin{aligned}&\mathbf{A}_{\mathbf{t}is}\mathbf{S}_{qs}+u_{qi}\mathbf{A}_{\mathbf{x}qp}\mathbf{S}_{pi}+v_{qi}\mathbf{A}_{\mathbf{y}qp}\mathbf{S}_{pi}-D_{s}\mathbf{B}_{\mathbf{x}qp}\mathbf{S}_{pi}-D_{s}\mathbf{B}_{\mathbf{y}qp}\mathbf{S}_{pi}=0\\&\mathbf{A}_{\mathbf{t}is}\mathbf{C}_{qs}+u_{qi}\mathbf{A}_{\mathbf{x}qp}\mathbf{C}_{\mathbf{p}i}+v_{qi}\mathbf{A}_{\mathbf{y}qp}\mathbf{C}_{pi}-D_{c}\mathbf{B}_{\mathbf{x}qp}\mathbf{C}_{pi}-D_{c}\mathbf{B}_{\mathbf{y}qp}\mathbf{C}_{pi}=0\end{aligned}\tag{67}$$

The formulation by OCFEM for element boundary conditions (fluxes at common collocations of adjacent elements is continuous) and boundary conditions can be done in the same way. Note that the same way is described for oxygen.

Element boundary condition(Element connection condition)：

$$\left(\left(u_r\mathbf{S}_r-D_{sf}\mathbf{A}_{\mathbf{x}rp}\mathbf{S}_p\right)l+\left(v_r\mathbf{S}_r-D_{sf}\mathbf{A}_{\mathbf{y}rp}\mathbf{S}_p\right)m\right)^{e1}-\left(\left(u_h\mathbf{S}_h-D_{sf}\mathbf{A}_{\mathbf{x}hp}\mathbf{S}_p\right)l+\left(v_h\mathbf{S}_h-D_{sf}\mathbf{A}_{\mathbf{y}hp}\mathbf{S}_p\right)m\right)^{e2}=0\tag{68}$$

Conditional expressions for the collocation of four corners within the region in the element boundary conditions (element connection conditions) is guided using the concept of least squares.

$$\begin{aligned}&\sum_{\substack{km=1\\ke=km}}^{m}\left\{\left(\left(u_r\mathbf{S}_r-D_{sf}\mathbf{A}_{\mathbf{x}rp}\mathbf{S}_p\right)l_{km}+\left(v_r\mathbf{S}_r-D_{sf}\mathbf{A}_{\mathbf{y}rp}\mathbf{S}_p\right)m_{km}\right)^{ke}-\left(\left(u_h\mathbf{S}_h-D_{sf}\mathbf{A}_{\mathbf{x}hp}\mathbf{S}_p\right)l_{km}+\left(v_h\mathbf{S}_h-D_{sf}\mathbf{A}_{\mathbf{y}hp}\mathbf{S}_p\right)m_{km}\right)^{ke+1}\right\}\\&\left\{\left(\left(u_r-D_{sf}A_{xrr}\right)l_{km}+\left(v_r-D_{sf}A_{yrr}\right)m_{km}\right)^{ke}-\left(\left(u_h-D_{sf}A_{xhh}\right)l_{km}+\left(v_h-D_{sf}A_{yhh}\right)m_{km}\right)^{ke+1}\right\}=0\end{aligned}\tag{69}$$

m：Number of elements sharing one corner, ke, $ke+1$：Elements and Adjacent Elements, km：Nodal edges through one of the four corners, r, h：Local number of shared collocations at the nodes of one element and adjacent elements.

Boundary condition：(refer to Fig.3) the same way is described for C.

① $S = S_0, \quad C = C_0$

② Boundary condition between Biofilm and Diffusion layer：

$$\left(u\mathbf{S}_r - D_{sf}\mathbf{A}_{\mathbf{x}rp}\mathbf{S}_p\right)l + \left(v\mathbf{S}_r - D_{sf}\mathbf{A}_{\mathbf{y}rp}\mathbf{S}_p\right)m = \left(u\mathbf{S}_h - D_s\mathbf{A}_{\mathbf{x}hp}S_p\right)l + \left(v\mathbf{S}_h - D_s\mathbf{A}_{\mathbf{y}hp}\mathbf{S}_p\right)m \tag{70}$$

③ On membrane：

$$D_{sf}\mathbf{A}_{\mathbf{x}rp}\mathbf{S}_p l + D_{sf}\mathbf{A}_{\mathbf{y}rp}\mathbf{S}_p m = 0 \tag{71}$$

④ $$\left(u\mathbf{S}_r - D_s\mathbf{A}_{\mathbf{x}rp}S_p\right)l + \left(v\mathbf{S}_r - D_s\mathbf{A}_{\mathbf{y}rp}\mathbf{S}_p\right)m = 0 \tag{72}$$

⑤ $$\left(u\mathbf{S}_r - D_{sf}\mathbf{A}_{\mathbf{x}rp}S_p\right)l + \left(v\mathbf{S}_r - D_{sf}\mathbf{A}_{\mathbf{y}rp}\mathbf{S}_p\right)m = 0 \tag{73}$$

Calculation of substrate consumption rate and flux by area and line integration

① Calculation of substrate consumption rate：

The substrate consumption rate of the biofilm can be calculated by integrating the specific substrate consumption rate at the collocation of each element of the biofilm (*S_Consum*). Since orthogonal collocations which are the roots of the Legendre polynomial are used for integral point, the Gauss-Legendre numerical integration formula for the area can be used with high-precision. The following is a specific numerical integration formula.

$$S\_Consum = \sum_{j=1}^{m}\sum_{i=5+4\cdot N}^{(N+2)(N+2)} \frac{v_{s\max}S_i^j}{K_S + S_i^j}\frac{C_i^j}{K_C + C_i^j} X_f W_i\left(\left(a_2 + a_4\eta_i\right)\left(b_3 + b_4\xi_i\right) - \left(a_3 + a_4\xi_i\right)\left(b_2 + b_4\eta_i\right)\right) \tag{74}$$

The above equation is described as a quadrilateral element.

② Calculation of inflow and outflow flux：

The flux of inflow and outflow on the surface of the biofilm is determined by linear integral. Gauss-Legendre's numerical integration formula can be used, and high-precision integration is possible.

$$Flux = \sum_{i=1}^{N} W_i f\left(x_i, y_i\right)\sqrt{a_2^2 + b_2^2} \tag{75}$$

Where

$$f\left(x_i, y_i\right) = \left(u_i S_i - D_{sf}\left.\frac{\partial S}{\partial x}\right|_i\right)l + \left(v_i S_i - D_{sf}\left.\frac{\partial S}{\partial y}\right|_i\right)m = \left(u_i\mathbf{S}_i - D_{sf}\mathbf{A}_{\mathbf{x}ip}\mathbf{S}_p\right)l + \left(v_i\mathbf{S}_i - D_{sf}\mathbf{A}_{\mathbf{y}ip}\mathbf{S}_p\right)m \tag{76}$$

The above equation describes the flux on the side of the quadrilateral element.

In the biofilm model, the substrate consumption rate and the flux balance of inflow and outflow must match at steady state.

Computational conditions and biofilm model parameters

The calculation conditions and the biofilm model parameter values in Table 1 used for numerical calculations are shown. Fig.5 and Fig.6 show examples of rectangular element division (Case1) and quadrilateral element division (Case2) in the case of 5×5 internal collocations in one element, respectively.

Calculation condition：

Substrate (Glucose) concentration in bulk liquid：10mg/l

Oxygen concentration in bulk liquid　　　　　　：4mg/l

Advection in the direction of y by membrane suction：-7μm/s

Space internal collocation in one element：2×2,　5×5,　7×7

Time internal collocation in time element：1, 2, 3, 4

Time element DT：0.01(when time collocation is 1),

0.1 (when time collocation is 2,3,4)

Total time of calculation.：20sec(steady state at 20sec)

Initial condition：Discontinuous initial conditions are given by using the initial concentration distribution in the diffusion layer and the biofilm as 1/2 of the concentration of the bulk liquid, and the upper boundary of the diffusion layer as the concentration of the bulk liquid.

Table 1 Parameter of biofilm model

parameter of biofilm model	symbol	parameter value
Diffusivity of substrate in Biofilm	D_{sf}	$0.25\times10^{-5}cm^2/sec$
Diffusivity of oxygen in Biofilm	D_{cf}	$1.37\times10^{-5}cm^2/sec$
Diffusivity of substrate in water	D_s	$0.694\times10^{-5}cm^2/sec$
Diffusivity of oxygen in water	D_c	$3.01\times10^{-5}cm^2/sec$
Maximum specific substrate removal rate	ν_{smax}	0.0002662 (1/sec)
Stoichiometric ratio of sbstrate and oxygen	α	0.5
Saturation constant of substrate	K_s	5mg/l
Saturation constant of oxygen	K_c	0.15mg/l
Density of bacteria in Biofilm	X_f	25000mg/l

Results and discussion in computation

Fig.6 and Fig.7 show the concentration profiles of the substrate (glucose) and oxygen in the biofilm models of the rectangular element (Case1) and the quadrilateral element (Case2) after the calculation time of 20 sec, respectively.

Fig.8 and Fig.9 show the concentration profiles of the substrate (glucose) and oxygen in the non-steady state after the calculation time of 1 sec in the biofilm model of the rectangular element (Case1) and the quadrilateral element (Case2), respectively. Although the initial conditions were spatially discontinuous, the concentration distribution after 1 sec (time element 0.01, time internal collocation 1) was shown to be stable with respect to space.

Fig.10 and Fig.11 show the total substrate consumption rate of the biofilm model in the unsteady state of the substrate (glucose) and oxygen in the biofilm model of the rectangular element (Case1), the total substrate flux flowing into the biofilm surface (inlet flux), and the total substrate flux flowing out of the membrane (outlet flux). and the change in flux balance of all substrate fluxes in and out over time. Before the aging time of 4 sec, the total substrate consumption rate (Consumption rate) and the flux balance (Flux balance) change non-stationarily and do not coincide, but after the aging change is 7 sec or more, the total substrate consumption rate and flux balance become a steady state, and the substrate consumption (unit time) consumed

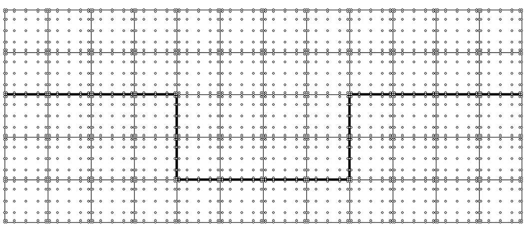


Fig.4 elements number:12×5 interior collocation（5×5＝25）
(Case1) Rectangular element in diffusion and biofilm domain

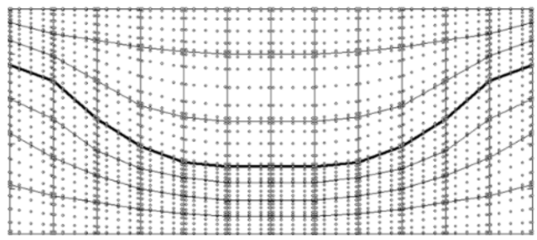
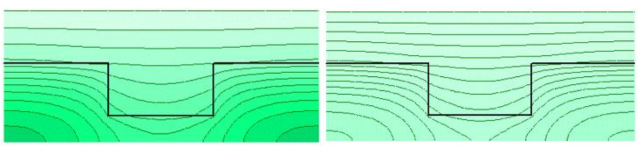
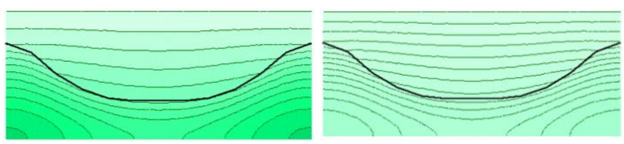


Fig.5 elements number:12×7 interior collocation（5×5＝25）
(Case2) Quadrilateral elements in diffusion and biofilm domain



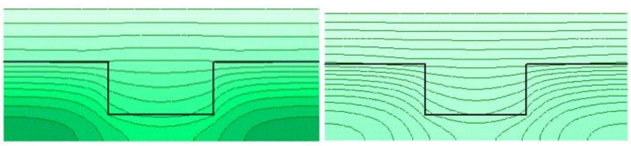
Substrate profile (interval 0.5mg/l) Oxygen profile (interval 0.05mg/l)

Fig.6 Steady profile of substrate and oxygen (after 20sec)
[Case 1:rectangular element（interior collocation 7×7）]



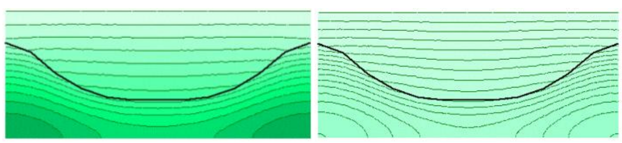
Substrate profile (interval 0.5mg/l) Oxygen profile (interval 0.05mg/l)

Fig.7 Steady profile of substrate and oxygen (after 20sec)
[Case 2:Quadrilateral element（interior collocation 7×7）]



Substrate profile (interval 0.5mg/l) Oxygen profile (interval 0.05mg/l)

Fig.8 Unsteady profile of substrate and oxygen (after 1sec)
[Case 1:rectangular element（interior collocation 7×7）]



Substrate profile (interval 0.5mg/l) Oxygen profile (interval 0.05mg/l)

Fig.9 Unsteady profile of substrate and oxygen (after 1sec)
[Case 2:Quadrilateral element（interior collocation 7×7）]

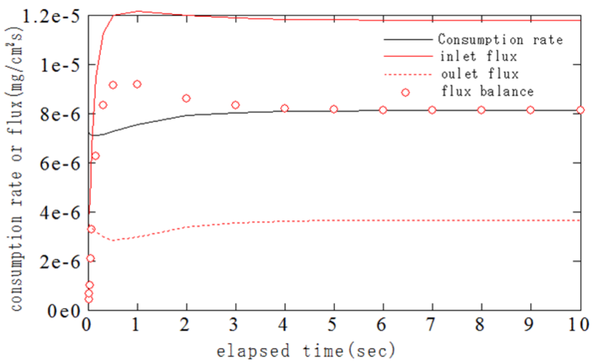


Fig.10 Time variation of consumption and flux balance of substrate (Case1: rectangular element) (time collocation 1) (interior collocation 7×7)

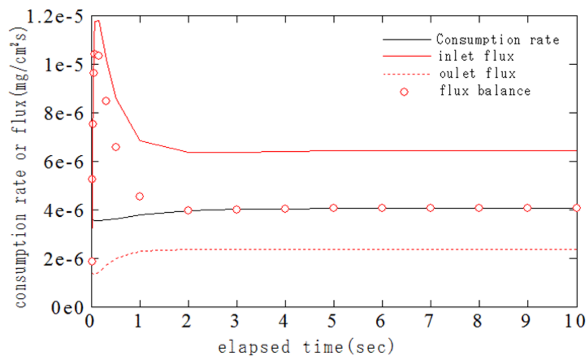


Fig.11 Time variation of consumption and flux balance of oxygen (Case1: rectangular element) (time collocation 1) (interior collocation 7×7)

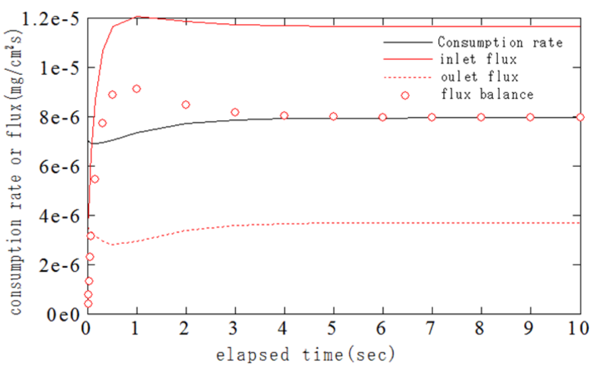


Fig.12 Time variation of consumption and flux balance of substrate (Case2: Quadrilateral element) (time collocation 1) (interior collocation 7×7)

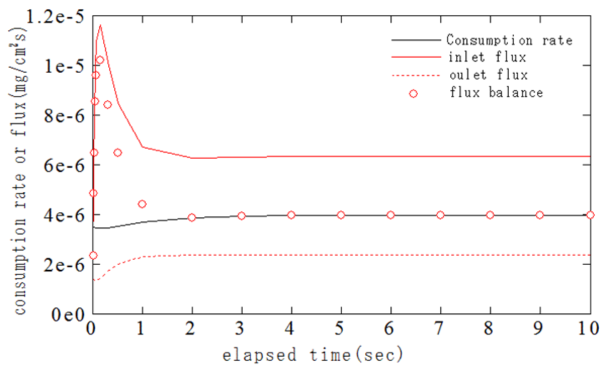


Fig.13 Time variation of consumption and flux balance of oxygen (Case2: Quadrilateral element) (time collocation 1) (interior collocation 7×7)

by the biofilm and the balance of the substrate mass (unit time) flowing into and outflowing into the biofilm coincide. It shows that the balance of substrates in steady state is consistent. Figs.12 and 13 show the changes in the consumption rate and flux balance of the substrate and oxygen over time in the biofilm model of quadrilateral elements, and show the same behavior as the biofilm model of rectangular elements. Fig.6~Fig.13 shows the calculation results when the number of internal collocations selected in the spatial element is 7×7 and the number of internal collocations in the time element (0.01) is 1.

Table 2 Unsteady and steady-state calculation values of substrate consumption rate and flux balance (time internal collocation number 1, time increment 0.01)(Unsteady calculation is the value in steady state (time 20s)) [Rectangular element: Case1]

substrate	substrate consumption rate (mg/s・cm²)	
internal collocation	unsteady calculation	steady calculation
2×2	8.121382663E-06	8.121382675E-06
5×5	8.121955997E-06	8.121956008E-06
7×7	8.121972148E-06	8.121972160E-06

substrate	flux balance (mg/s・cm²)	
internal collocation	unsteady calculation	steady calculation
2×2	8.121382702E-06	8.121382675E-06
5×5	8.121956035E-06	8.121956008E-06
7×7	8.121972187E-06	8.121972160E-06

Table 3 Effect of the number of internal collocations in time on the convergence of substrate consumption rate and flux at 0.5 sec.(Number of collocations in the space: 7×7, Biofilm morphology [Rectangular element: Case1])

time internal collocation	substrate consumption rate	biofilm surface flux	membrane outflow flux
1	7.269323411E-06	1.196666138E-05	2.834574954E-06
2	7.268561257E-06	1.197539826E-05	2.832248287E-06
3	7.268569034E-06	1.197526570E-05	2.832236852E-06
4	7.268569198E-06	1.197526671E-05	2.832237129E-06

Table 4 Effect of the number of internal collocations in time on the convergence of substrate consumption rate and flux balance in steady state (20 seconds)[Rectangular elements: Case1]

time internal collocation	substrate consumption rate	flux balance
1	8.121972149E-06	8.121972187E-06
2	8.121972149E-06	8.121972187E-06
3	8.121972149E-06	8.121972187E-06
4	8.121972149E-06	8.121972187E-06

The effects of the space and time collocations (time element 0.01: time internal collocation 1, time element 0.1: time internal collocation 2, 3, and 4) on the substrate consumption rate and flux convergence behavior are described using Table 2~Table 7. Table 2 shows the convergence of the calculated values of the non-stationary PDEs and stationary PDEs of the substrate consumption rate and flux balance numerically calculated by the number of internal collocations in space, and the convergence to a certain value is observed. It is shown that the steady-state value of non-stationary PDEs (after 20 sec) and the calculated value of stationary PDEs match up to 7 significant digits. Table 3 shows the effect of the number of internal collocations of time on the convergence of substrate consumption rate and flux after 0.5 seconds in numerical calculations of non-stationary PDEs, and shows that the consumption rate and flux converge as the number of internal points of time increases.

Table 4 shows the effect of the number of internal collocations of time on the convergence of the substrate consumption rate and flux balance in the steady state (after 20 seconds) of non-stationary PDEs, and it can be seen that the calculated values of the substrate consumption rate and flux do not depend on the number of time collocations. The substrate consumption rate and flux balance in steady state are consistent up to 8 significant digits.

Table 5 Unsteady and steady-state calculation values of substrate consumption rate and flux balance (time internal collocation number 1, time increment 0.01)(Unsteady calculation is the value in steady state (time 20s)) [Quadrilateral elements: Case2]

substrate	substrate consumption rate (mg/s・cm ^{2})	
internal collocation	unsteady calculation	steady calculation
2×2	7.945250017E-06	7.945250025E-06
5×5	7.945368876E-06	7.945368884E-06
7×7	7.945372917E-06	7.945372926E-06

substrate	flux balance (mg/s・cm ^{2})	
internal collocation	unsteady calculation	steady calculation
2×2	7.945249985E-06	7.945249965E-06
5×5	7.945368844E-06	7.945368823E-06
7×7	7.945372886E-06	7.945372865E-06

Table 6 Effect of the number of internal collocations in time on the convergence of substrate consumption rate and flux at 0.5 sec.(Number of collocations in the space: 5×5, Biofilm morphology [Quadrilateral elements: Case2])

time internal collocation	substrate consumption rate	biofilm surface flux	membrane outflow flux
1	7.037619540E-06	1.165297510E-05	2.794081582E-06
2	7.037597629E-06	1.165325589E-05	2.794064515E-06
3	7.037605746E-06	1.165312835E-05	2.794052791E-06
4	7.037605915E-06	1.165312908E-05	2.794053100E-06

Table 7 Effect of the number of internal collocations in time on the convergence of substrate consumption rate and flux balance in steady state (20 seconds)[Quadrilateral elements: Case2]

time internal collocation	substrate consumption rate	flux balance
1	7.945368876E-06	7.945368844E-06
2	7.945368876E-06	7.945368844E-06
3	7.945368876E-06	7.945368844E-06
4	7.945368876E-06	7.945368844E-06

Table 5~Table 7 is a model of quadrilateral elements, and in terms of content, it shows the same trend as the rectangular element model in Table 2~Table 4. However, Table 7 shows the case of spatial internal collocations 5×5, and the substrate consumption rate, which is the steady value of the non-stationary PDEs, and the flux balance were consistent up to 8 significant digits.

From the above, it is considered that the meaning of Weierstrass's theorem [(20)(23)] of polynomial approximation and the approximation of partial derivatives of polynomials (extension of Weierstrass's theorem) is that they converge uniformly when the order of the polynomial approximation (the order of the internal collocations) that approximates the unknown function to be found is increased. This cannot be said accurately because it has not been mathematically proven, but it is thought that it can be inferred that the tendency is to converge when the order of the polynomial (the number of internal points) is increased. Therefore, the differential operator of the orthogonal collocation finite element method is considered to be one of the important analysis methods for numerical analysis because it has a mathematical meaning.

Conclusions

The following findings were obtained from the formulation of the biofilm model using OCFEM, the numerical calculation of the concentration distribution, and the calculation of the substrate consumption rate and flux balance at the boundary of the biofilm region as a numerical integration of the concentration distribution.

① The formulation of the biofilm model using the differential operator (matrix) of OCFEM yielded the results of a reasonable concentration distribution, and the numerical integration of the concentration distribution of the biological region and the boundary yield yielded a reasonable substrate consumption rate and flux balance in the boundary region.

② By using a higher-order differential operator (matrix) with the order of the polynomial representation of the concentration in space, we were able to show the convergence of the substrate consumption rate and flux balance, which is the integral of the concentration distribution.

③ The consistency between the substrate consumption rate and the flux balance at the biofilm boundary, which is the integral of the steady-state value (concentration distribution) of the non-stationary PDEs and the calculation result (concentration distribution) of the stationary PDEs, was accurately consistent, and when the order of the time collocation in the nonstationary case (assuming that the time-related differential operator (matrix) was of a higher order) increase, the integral value of the substrate consumption rate and the flux balance converged to a certain value.

④ Numerical calculations of OCFEM have shown that Weierstraßs theorem of polynomial approximation and the approximation of partial derivatives of polynomials converge at each point by increasing the order of the polynomial (order of internal collocations: order of differential operator (matrix)) that approximates the unknown function to be obtained. By making it higher order (mathematically close to ∞), the arrangement of the orthogonal collocations becomes dense and can be expected to converge uniformly.

The above results can be inferred from the numerical calculations of OCFEM, and it goes without saying that they must be strictly proved mathematically, but from an engineering point of view, the practical use of OCFEM and potential is considered to be high.

Acknowledgement

I would like to express my sincere gratitude to the students of the Okubo Laboratory at that time, who spared no effort in the calculations using the OCFEM program.

Reference

(1) By B.A. Finlayson, Translated by Washizu and Yamamoto and Kawai, Weighted Residual Method and Variational Principle, in Japanese Baifukan, 1972

(2) Larry C. Young, Orthogonal collocation revisited, Comput. Methods Appl. Mech. Engng, 345(2019) 1033-1076

(3) J.V. Villadsen and W.E. Stewart, Solution of boundary-value problems by orthogonal collocation, Chem. Engng Sci. 22, 1483-1501, 1967

(4) Takaki Ohkubo, Formulation of Unsteady Two-Substrate Limitted Advection Diffusion Reaction Equation (Biofilm Model) by Orthogonal Collocation Finite Element Method and Calculation of Substrate Consumption and Flux, in Japanese, annual Meeting of the Japan Society for Industrial Mathematics, 2019.6

(5) G.F. Carey and Bruce A. Finlayson, Orthogonal collocation on finite elements, Chem. Engng Sci., 1975. Vol.30 pp. 587-596

(6) Bruce A. Finlayson, Orthogonal collocation on finite elements -Progress and potential, Math. And Comp. in Simu. XXⅡ(1980) 11-17

(7) Jacob H. Masliyah and Dileep Kumer, Application of orthogonal collocation on finite elements to a flow problem, Math. And Comp. in Simu.XXⅡ(1980) 49-54

(8) Laura Gardini, Use of orthogonal collocation on finite elements with moving boundaries for fixed bed catalytic reactor simulation, Comp. & Chem. Engng Vol.9, No.1, pp1-17, 1985

(9) Z. Ma and G. Guiochon, Application of orthogonal collocation on finite elements in the simulation of non-linear chromatography, Comp. Chem. Engng, Vol.15, No.6, pp. 415-426, 1991

(10) Shelly Arora, S.S. Dhaliwal, V.K. Kukreja, Solution of two point boundary value problem using orthogonal collocation on finite elements, Math. Comput. 171(2005) 358-370

(11) Shelly Arora, S.S. Dhaliwal, V.K. Kukreja, Application of orthogonal collocation on finite elements for solving non-linear boundary value problems, Applied and Computation 180(2006) 516-523

(12) Takaki Ohkubo, Effect of Improvement on Orthogonal Collocation Finite Element Method － On Nonlinear Advective-Diffusive-Reactive Equation of Two Substrate Limit－, in Japanese, abstract in English, Proceedings of Computational Engineering Conference Vol. 20 (June 2015)

(13) Takaki Ohkubo, Mathematical analysis of Advection-Diffusion-Reaction Equation by Orthogonal Collocation Finite Element Method, in Japanese, abstract in English, Proceedings of the Conference on Computational Engineering Vol. 21 (June 2016)

(14) Takaki Ohkubo, Numerical analysis of 2-dimensional unsteady equation of heat conduction by orthogonal collocation finite element method, in Japanese, abstract in English, Proceedings of the Conference on Computational Engineering Vol.21 (June 2016)

(15) Takaki Ohkubo, Calculation of Substrate Consumption Rate and Flux on Orthogonal Collocation Finite Element Method－On Nonlinear Advection-Diffusion-Reaction Equation of Two Substrate Limit－, in Japanese, abstract in English, Proceedings of Computational Engineering Conference Vol.23(June 2018)

(16) Takaki Ohkubo, On orthogonal collocation finite element method (OCFEM)－Progress direction and potential －In Japanese, abstract in English, Proceedings of Computational Engineering Conference Vol. 24(May 2019)

(17) Takashi Mikami, A Study on Analysis of Dynamic Problems of Structures by the Collocation Method, in Japanese, Ph.D. Dissertation, Hokkaido University, March 25, 1987

(18) Tetsuro Inui, Special Functions, in Japanese, Iwanami Zensho 252, June 30, 1966 3rd printing

(19) Takahiro Hasegawa, A Study on Improving the Accuracy of the Orthogonal Collocation Method and Its Application to Chemical Engineering Problems, Ph.D. Thesis, in Japanese, Kyushu Institute of Technology, February 14, 1997, Shizuoka Academic Publishing Co., Ltd. ISBN 978-4-903859-77-4

(20) Hisashi Okamoto and Ryosuke Nagaoka, What is a function?: An approach from the history of modern mathematics, in Japanese　pp.180-p188, 2014, Modern Science Co., Ltd.

(21) Norikazu Saito, Kyoritsu Lecture Mathematics Exploration Vol.17 Numerical Analysis, in Japanese, pp. 54-p66, 2017, Kyoritsu Shuppan

(22) Takaki Ohkubo, Formulation and numerical calculation of Biofilm model by differential operator of time and space in orthogonal collocation finite elements method, free paper

(23) Tetsuji Tokihiro, Engineering Mathematics Course 13 Special Functions in Engineering, Kyoritsu Publishing Co., Ltd., 2006 , in Japanese