

CCFD

Theoretical Manual

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Contents

1.	Introduction	1
1.1.	CCFD.....	1
1.2.	Using this Manual.....	2
2.	Mathematical Models	3
2.1.	Governing Equations	3
2.1.1	Law of Conservation of Mass.....	3
2.1.2	Law of Conservation of Momentum	4
2.1.3	Energy Equations	5
2.1.4	Law of Conservation of Space.....	5
2.1.5	Non-Newtonian Fluids	5
2.2.	Turbulent Model.....	5
3.	Numerical Analysis Method	9
3.1.	Mathematical Model.....	9
3.2.	Discretization Method.....	10
3.2.1	Geometric Approximation	11
3.2.2	Integration Calculation	11
3.2.3	Interpolation Method.....	11
3.3.	Derivation of Algebraic Equations	12
3.3.1	Unsteady Terms	12
3.3.2	Advective Terms.....	12
3.3.3	Diffusion Terms.....	13
3.3.4	Source Terms.....	13
3.3.5	Boundary Conditions	14
3.3.6	Algebraic Equations	14
3.3.7	Pressure Compensation Calculations	15
3.4.	Algorithms	16
3.4.1	SIMPLE algorithm.....	16
3.4.2	Under-relaxation	17
3.4.3	SMAC algorithm.....	17
3.5.	Boundary Conditions	18
3.5.1	Wall Conditions	18
3.5.2	Natural Outflow	19
3.5.3	Inflow Conditions	19
3.5.4	Temperature Boundary (chemical species).....	19

1. Introduction

1.1. CCFD

The CCFD is thermohydrodynamic analysis code that embodies fluid analysis technology developed by CRC Solutions (Inc.) over many years. This is analysis code of complete non-structural lattices developed for the purpose of fluidic / structural coupled analysis using the general-purpose FEM nonlinear structural analysis system FINAS. The CCFD calculates the heat and flow of air and fluid and then allows the mutual interaction of fluids and structural shapes to be calculated by passing the calculation results to FINAS.

Calculations can be performed with non-structural lattices by means of using a finite volume method that uses a Gauss divergence theorem to perform discretization on intact governing equations described by integral calculus expressions. This makes it possible to perform calculations using calculation lattices which resemble finite element method lattice partitions as well as create data without being aware of calculation lattices used for thermohydrodynamic analysis and calculation lattices used for structural analysis.

Outline

- Allows partitioning of complete non-structural lattices that correspond to hexahedrons and tetrahedral elements, and the partition the elements that match the shapes by means of using a finite volume method that separates intact a Navier-Stokes equation described by an integral equation.
- Allows use of general-purpose nonlinear structural analysis system FINAS to perform fluidic / structural coupled analysis.
- Allows efficient calculations with simple algorithms by means of using analysis through collocated grids that inhibit numerical value oscillations.

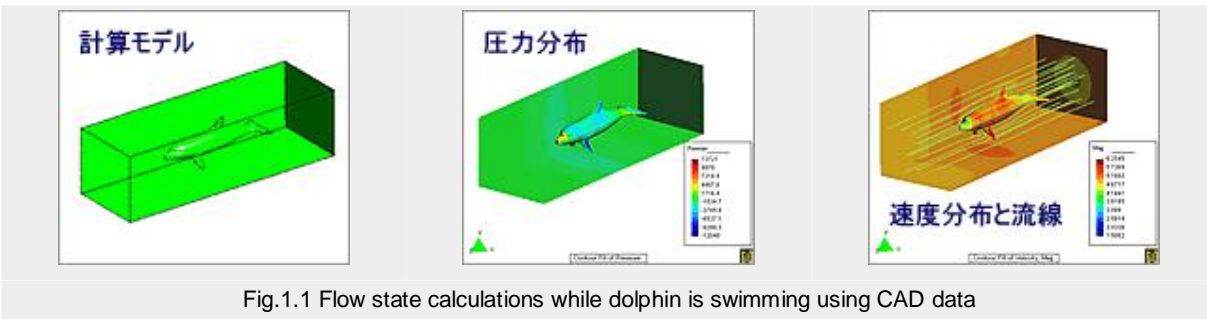
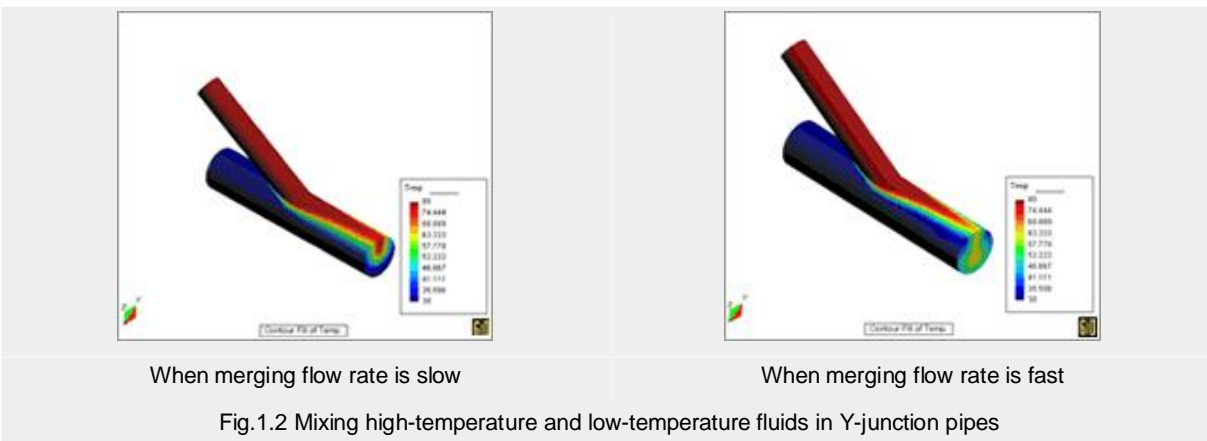


Fig.1.1 Flow state calculations while dolphin is swimming using CAD data

Construction of compound field analysis system

- Allows coupled analysis between electromagnetic fields with a simple construction through the use of a design that takes into consideration coupling between fields other than fluids.
- Allows structural analysis and calculations of lattices identical to electromagnetic field analysis through the use of meshing partitions that use complete non-structural lattices.



When merging flow rate is slow

When merging flow rate is fast

Fig.1.2 Mixing high-temperature and low-temperature fluids in Y-junction pipes

2. Mathematical Models

This section describes items related to mathematical models in physical phenomenon calculated by the CCFD.

2.1. Governing Equations

The conservation laws related to the following items for calculating thermal hydraulic phenomenon are considered in the CCFD.

- Mass
- Momentum
- Energy
- Other (scalar variables)

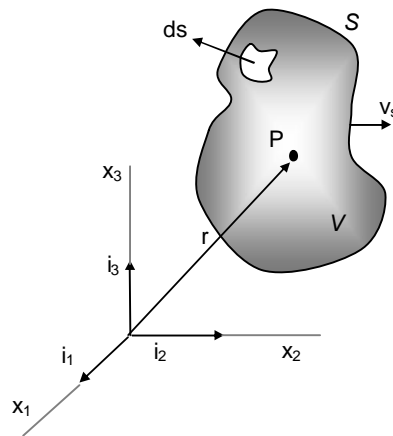


Fig. Control Volume

Here, governing equations are described by integral calculus expressions using cubic volume V surrounded by surface area S for equations that represent the conservation law mentioned above. In addition, v_s here is the transfer velocity of the boundary. When v_s is the same as velocity v of the continuum, it is described by a Lagrangian form and when $v_s = 0$, a Eulerian form.

2.1.1 Law of Conservation of Mass

Equation of continuity

The law of conservation of mass is known as an equation of continuity and is represented by the following equation.

$$\frac{d}{dt} \int_V \rho dV + \int_S \rho (v - v_s) \cdot ds = 0 \quad (2.1)$$

Here, ρ is density and s is a value of an outward normal vector multiplied by a surface area.

Equation of chemical species conservation

When certain chemical species are mixed, variables representing each of the chemical species must satisfy the following equation.

$$\frac{d}{dt} \int_V \rho c_i dV + \int_S \rho c_i (v - v_s) \cdot ds = \int_S q_{c_i} \cdot ds + \int_V s_{c_i} dV \quad (2.2)$$

Here, c_i is a variable representing a chemical species or a mass fraction represented by the following equation.

$$c_i = \frac{m_i}{m} \quad (2.3)$$

Here, m_i is the mass of an i th chemical species and m is the mass of a certain point.

In addition, q_{c_i} is the diffusion and s_{c_i} is a source term.

c_i from the definition of equation (2.3) satisfies the following equation.

$$\sum_{i=0}^N c_i = 1 \quad (2.4)$$

If the Fick law is used, the following relationship is derived.

$$q_{c_i} = \rho c_i (v_{c_i} - v) \quad (2.5)$$

Here, v_{c_i} is the i th velocity and is $v = \sum_{i=0}^N c_i v_{c_i}$. For this the relationship with the diffusion shown below is obtained.

$$q_{c_i} = \rho D_i \text{grad} c_i \quad (2.6)$$

This is diffusion of D_i mass here.

2.1.2 Law of Conservation of Momentum

By means of applying Newton's 2nd law to the control volume of Fig. 2.1, the following equation is derived known as Cauchy's 1st law of motion.

$$\frac{d}{dt} \int_V \rho v dV + \int_S \rho v (v - v_s) \cdot ds = \int_S T \cdot ds + \int_V f_b dV \quad (2.7)$$

Here, T is a Cauchy stress tensor and f_b is the volume force per unit volume.

If Stokes' law is used, the following equation is obtained.

$$T = 2\mu \dot{D} - \frac{2}{3} \mu \text{div} v I - p I \quad (2.8)$$

Here, we derive the following equation.

$$\dot{D} = \frac{1}{2} [\text{grad} v + (\text{grad} v)^T] \quad (2.9)$$

Here, μ is the viscosity coefficient of the fluid, p is the pressure, and I the unit tensor.

2.1.3 Energy Equations

$$\frac{d}{dt} \int_V \rho e dV + \int_S \rho e (v - v_s) \cdot ds = \int_S q_h \cdot ds + \int_V s_h dV \quad (2.10)$$

Here, q_h is a heat flux vector and s_h is a heat source.

If Fourier's law is used, the following equation is obtained.

$$q_h = \kappa \text{grad} T \quad (2.11)$$

Here, κ is the thermal conductivity.

2.1.4 Law of Conservation of Space

The law of conservation of space is considered when transferring a boundary.

$$\frac{d}{dt} \int_V dV - \int_S v_s \cdot ds = 0 \quad (2.12)$$

2.1.5 Non-Newtonian Fluids

This is an Ostwald-de Waele or power law model.

$$T = 2\mu_0 |\Pi_D|^{\frac{n-1}{2}} \dot{D} - pI \quad (2.13)$$

Here, we derive the following equation.

$$\Pi_D = \frac{1}{2} \dot{D} : \dot{D} \quad (2.14)$$

2.2. Turbulent Model

The CCFD is provided with a standard k- ϵ model and LES (Large Eddy Simulation) as turbulent models. Each model is described below.

Standard k- ϵ model

A standard k- ϵ model is a model often used effectively as an eddy viscosity model. D_i , μ , and κ in equations (2.6), (2.8), and 2.11) are used as values that take turbulent flow into consideration.

$$\begin{aligned} D_{i,eff} &= D_i + D_{i,t} \\ \mu_{eff} &= \mu + \mu_t \\ \kappa_{eff} &= \kappa + \kappa_t \end{aligned} \quad (2.15)$$

Here, $\rho D_{i,t}$, μ_t , and κ_t are turbulent mass diffusion coefficients, eddy viscosity coefficients, and turbulent conduction coefficients, respectively. They are represented by the following equation.

$$\rho D_{i,t} = \frac{\mu_t}{\sigma_{c_i}} \mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \kappa_t = \frac{\mu_t C_p}{\sigma_T} \quad (2.16)$$

Turbulent kinetic energy k and eddy dispersion rate ε are modeled by the following transport equations.

$$\frac{d}{dt} \int_V \rho k dV + \int_S \rho k (v - v_s) \cdot ds = \int_S q_k \cdot ds + \int_V (P + P_B - \rho \varepsilon) dV \quad (2.17)$$

$$\begin{aligned} & \frac{d}{dt} \int_V \rho \varepsilon dV + \int_S \rho \varepsilon (v - v_s) \cdot ds \\ & = \int_S q_\varepsilon \cdot ds + \int_V \left(C_1 P \frac{\varepsilon}{k} - C_2 \rho \frac{\varepsilon^2}{k} + C_3 \max(P_B, 0) \frac{\varepsilon}{k} - C_4 \rho \varepsilon \operatorname{div} v \right) dV \end{aligned} \quad (2.18)$$

Here, the flux of turbulent kinetic energy k and eddy dispersion rate ε are represented as shown below.

$$q_k = \left(\mu + \frac{\mu_t}{\sigma_k} \right) \operatorname{grad} k, \quad q_\varepsilon = \left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \operatorname{grad} \varepsilon \quad (2.19)$$

Furthermore, turbulent kinetic energy P generated by shear and the effect P_B due to buoyancy are modeled as shown below.

$$P = T_t : \operatorname{grad} v = 2\mu_t \dot{D} : \dot{D} = \frac{2}{3} (\mu_t \operatorname{div} v + \rho k) \operatorname{div} v \quad (2.20)$$

$$P_B = -\frac{\mu_t}{\rho \sigma_T} g \cdot \operatorname{grad} \rho \quad (2.21)$$

Here, $C_1, C_2, C_3, C_4, \sigma_k, \sigma_\varepsilon, \sigma_T$ are experimental constants and use the values in Table 2.1

Table 2.1 Standard k-ε model experimental constants

C_μ	C_1	C_2	C_3	C_4	σ_k	σ_ε	σ_T	σ_{c_i}
0.09	1.44	1.92	1.44	-0.33	1.0	1.3	0.9	0.9

LES model

The following equation considers the local spatial average of physical quantity $f(r, t)$ (function of time and space).

$$\bar{f}(r, t) = \int_{\infty} G(r, r') f(r', t) dr' \quad (2.22)$$

Here, $G(r, r')$ is a filter function and several functions are proposed.

The following equation is obtained if filtering of a Navier-Stokes equation (2.22) is performed for incompressible fluid.

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (2.23)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial}{\partial x_j} (\overline{u_i' u_j'} - \overline{u_i' u_j'}) \quad (2.24)$$

In equation (2.23), besides the original Navier-Stokes equation, the additional terms shown below appear in unknown quantities \bar{u}_i , \bar{p} of large-scale quantities.

$$\overline{u_i u_j} - \overline{u_i} \overline{u_j} = L_{ij} + C_{ij} + R_{ij} \quad (2.25)$$

$$L_{ij} = \overline{\overline{u_i u_j}} - \overline{u_i} \overline{u_j} \quad (2.26)$$

$$C_{ij} = \overline{u_i' u_j'} + \overline{u_i' u_j} \quad (2.27)$$

$$R_{ij} = \overline{u_i' u_j'} \quad (2.28)$$

L_{ij} , C_{ij} , R_{ij} are apparent stress on large-scale eddy locations occurring due to the filtering. Each one is called a Leonard term, Cross term, and Reynolds term, respectively.

SGS model

Ignores a Leonard term and a Cross term and then applies an SGS model to a Reynolds term.

Thereafter, the following equation is given to a table expression of molecular viscosity viscous friction.

$$R_{ij} = \overline{u_i' u_j'} - \delta_{ij} \overline{u_k' u_k'} / 3 = -\nu_T \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (2.29)$$

As shown in the equation below, transport energy of a small-scale eddy can also be obtained from equation (2.24) in the procedure that derives a transport equation of eddy stress used in a Reynolds averaging equation.

$$k_s = \overline{u_k' u_k'} / 2 = (\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) / 2 \quad (2.30)$$

In other words, the right side of equation (2.31) is the generation term, the turbulent diffusion term, and the dispersion term (ε_s).

$$\frac{\partial k_s}{\partial t} + \bar{u}_j \frac{\partial k_s}{\partial x_j} = -\frac{1}{2} R_{ij} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{\partial}{\partial x_j} \left(\frac{1}{2} \overline{u_j' u_k' u_k'} + \frac{1}{\rho} \overline{p' u_j'} + \nu \frac{\partial^2 k_s}{\partial x_k^2} - \nu \left(\frac{\partial u_i'}{\partial x_k} \right)^2 \right) \quad (2.31)$$

If $k_s^{1/2}$ is a representative value of velocity and we select a representative value Δ of length, the following equation can be expressed from dimensional analysis.

$$\varepsilon_s \approx k_s^{3/2} / \Delta \quad (2.32)$$

$$\nu_T \approx (\varepsilon_s \Delta^4)^{1/3} \quad (2.33)$$

If the generation term and the dispersion term are significantly large and these two terms are approximated to be in proportion in equation (2.31), the following equation is obtained.

$$\nu_T = (C_s \Delta)^2 \sqrt{2\bar{D}} \quad (2.34)$$

Here, the following relationships exist.

$$D_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (2.35)$$

$$\bar{D} = (\bar{D}_{ij} \bar{D}_{ij})^{1/2} \quad (2.36)$$

Δ is a representative value of filter width in a cube lattice. It is also the distance of the wall and center of the cell close to the wall. C_s is called a Smagorinsky constant and is often values between 0.085 to 0.11.

3. Numerical Analysis Method

This section describes details of numerical analysis method used in the CCFD.

3.1. Mathematical Model

Except for the law of conservation of mass, the law of conservation of momentum, the law of conservation of energy, and the governing equation related to the turbulent (k-ε) model considered in the CCFD are uniformly described as shown below.

$$\frac{d}{dt} \int_V \rho B_\phi dV + \int_S \rho \phi (v - v_s) \cdot dS = \int_S \Gamma_\phi \text{grad} \phi \cdot dS + \int_S q_{\phi S} \cdot dS + \int_V q_{\phi V} dV \quad (3.1)$$

Here, ϕ represents a dependent variable that should be solved for velocity with a Navier-Stokes equation. In addition, when ϕ is a scalar quantity, it can be handled as temperature and density using boundary conditions. Each symbol in equation (2.1) has the following meaning. s is an outward surface vector.

Table 3.1 Variables

ϕ	B_ϕ	Γ_ϕ	$q_{\phi S}$	$q_{\phi V}$
c_i	c_i	$\rho D_{i,eff}$	0	s_{ci}
v_i	v_i	μ_{eff}	$\left[\mu_{eff} (\text{grad} \mathbf{v})^T - \left(\frac{2}{3} \mu_{eff} \text{div} \mathbf{v} + p \right) \mathbf{I} \right] \cdot \mathbf{i}_i$	$f_{b,i}$
e	e	$\frac{\kappa}{\partial e / \partial T} + \frac{\mu_t}{\sigma_T}$	$-\frac{\kappa}{\partial e / \partial T} \frac{\partial e}{\partial p} \text{grad} p$	$T : \text{grad} \mathbf{v} + s_h$
k	k	$\mu + \frac{\mu_t}{\sigma_k}$	0	$P + P_B - \rho \varepsilon$
ε	ε	$\mu + \frac{\mu_t}{\sigma_\varepsilon}$	0	$C_1 P \frac{\varepsilon}{k} - C_2 \rho \frac{\varepsilon^2}{k} +$ $C_3 \max(P_B, 0) \frac{\varepsilon}{k} - C_4 \rho \varepsilon \text{div} \mathbf{v}$

The CCFD uniformly handles values such as velocity, temperature, turbulent energy (k), and eddy dispersion rate (ε) by performs discretization using the format of equation (3.1). The CCFD is also designed with more efficient calculations and improved flexibility for the number variables that can be handled.

3.2. Discretization Method

The CCFD utilizes a finite volume method that performs discretization on intact equations described by integral calculus expressions for the purpose of using non-structural lattices to perform precision calculations. The advantages of using a finite volume method are shown below.

- Can handle polyhedrons.
- Discretization using non-structural lattices
- Can define all variables in center of a cell by means of using a collocated grid for more efficient calculations.

The CCFD uses a collocated grid to arranged variables in center of a cell. If we use the symbols of Fig. 3.1, equation (2.1) will be described as shown below.

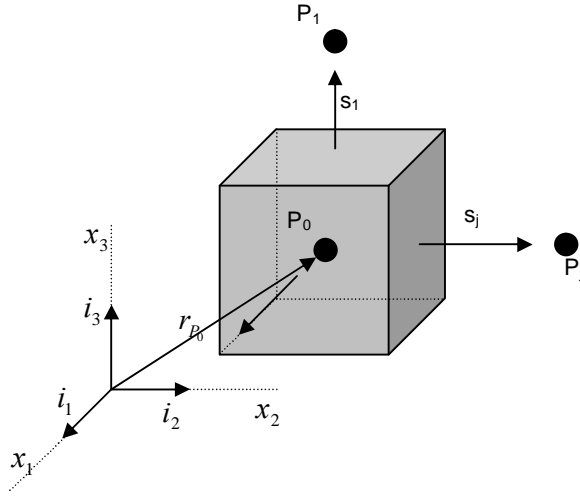


Fig.3.1 Variable arrangement

$$\frac{d}{dt} \int_V \rho B_\phi dV + \sum_{j=1}^{n_f} \int_{S_j} \rho \phi (v - v_s) \cdot ds = \sum_{j=1}^{n_f} \int_{S_j} \Gamma_\phi \text{grad} \phi \cdot ds + \sum_{j=1}^{n_f} \int_{S_j} q_{\phi S} \cdot ds + \int_V q_{\phi V} dV \quad (3.2)$$

Here, n_f is the number of surfaces comprising a cell.

The first term on the left side of equation (3.2) is an unsteady term and the second term is an advective term. The first term on the right side is a diffusion term and the second and third terms are both source terms.

The following procedure is completed in order to evaluate the integral terms appearing in equation (3.2).

- a) Shape data processing to calculate the surface integral and cubic volume integral
- b) Select approximation method of cubic volume integral
- c) Select interpolation method of variables
- d) Select discretization method for advective terms
- e) Select integral scheme
- f) Calculate velocity of cell interface

These calculation methods are shown below.

3.2.1 Geometric Approximation

A surface integral and a cubic volume integral for dependent variables are required when performing discretization on integral equations. The surface area of the cell and cubic volume values are also required. These calculation methods are shown below.

Outward surface vector

Uses the following approximation to calculate the surface area of the cell in equation (3.2).

$$s_j = \frac{1}{2} \sum_{i=3}^{n_j^v} |(r_{i-1} - r_1) \times (r_i - r_1)| \quad (3.3)$$

Here, n_j^v is the value of an articulation point comprising surface j and r_i is a position vector of articulation point i .

Cell cubic volume

Uses the following approximation to calculate the cubic volume of the cell in equation (3.2).

$$\int_V \text{div } r \, dV = \int_S r \cdot ds \Rightarrow V_{P_0} = \frac{1}{3} \sum_{j=1}^{n_f} r_j \cdot s_j \quad (3.4)$$

Here, r_i is a position vector towards the center of surface j comprising the cell.

3.2.2 Integration Calculation

Uses the approximation shown in 2.2.1 to calculate the integral for each term in equation (3.2) as shown below.

$$\int_{S_j} f \cdot ds \approx f \cdot s_j, \quad \int_V f dV \approx f_{P_0} V_{P_0} \quad (3.5)$$

Here, f represents an arbitrary scalar and vector variable.

3.2.3 Interpolation Method

Calculations in equation (3.2) require values at the cell boundary. This method basically uses the values at the center of the cell and the values located at arbitrary positions are then found as shown below.

$$\Psi(r) = \Psi_{P_0} + (\text{grad}\Psi)_{P_0} \cdot (r - r_{P_0}) \quad (3.6)$$

Here, P_0 is an identifier that represents the value at the center of the cell and r is a position vector of the location whose value you want to find.

Based on equation (3.6), the CCFD uses equations to which revisions for a collocated grid are added to calculate values on surfaces.

Values on cell surface

$$\psi_j = \frac{1}{2}(\psi_{P_0} + \psi_{P_j}) + \frac{1}{2} \left[(\text{grad}\psi)_{P_0} \cdot (r_j - r_{P_0}) + (\text{grad}\psi)_{P_j} \cdot (r_j - r_{P_j}) \right] \quad (3.7)$$

Here, r_i is a position vector towards the center of the cell and P_j is an identifier of the adjacent cell. The first term on the right side is a value at the center point when center P_0 and center P_j are linked using a straight line. The second term is a revised value when the center point within the center is not located at the center the cell surface.

Gradient calculations

The CCFD uses the following equation according to the Gauss theory as a calculation of the gradient at the center of the cell.

$$\int_V \text{grad}\psi dV = \int_S \psi dS \Rightarrow (\text{grad}\psi)_{P_0} \approx \frac{1}{V_{P_0}} \sum_{j=1}^{n_f} \psi_j s_j \quad (3.8)$$

Here, ψ_j represents the value of ψ at the center of the cell surface j .

3.3. Derivation of Algebraic Equations

The CCFD uses a SIMPLE method as a solution method of equation (3.2). The linear simultaneous equation derived when applying a SIMPLE method is as follows.

3.3.1 Unsteady Terms

In the CCFD the unsteady terms of equation (3.2) use an implicit method of first order precision to perform discretization as shown below.

$$\frac{d}{dt} \int_V \rho B_\phi dV \approx \frac{(\rho B_\phi V)_{P_0} - (\rho B_\phi V)_{P_0}^{m-1}}{\delta t_m} \quad (3.9)$$

Here, ρ is density, B is a dependent variable, and δt_m is a time unit.

3.3.2 Advective Terms

The flux of variable ϕ that passes through the cell surface is as shown in the following equation.

$$C_j = \int_{S_j} \rho \phi (v - v_s) \cdot ds \approx \dot{m}_j \phi_j^* \quad (3.10)$$

Here, ϕ_j^* represents the value at the center of the surface comprising the cell and \dot{m}_j is the mass flux on the surface of the cell derived by the following equation.

$$\dot{m}_j = \int_{S_j} \rho (v - v_s) \cdot ds \approx \rho_j^* (v_j^* \cdot s_j - \dot{V}_j) \quad (3.11)$$

ρ_j^* , v_j^* are described later.

The CCFD is provided with the following two types of discretization skim of advective terms.

First order upwind

$$\phi^{UD} = \begin{cases} \phi_{P_0}, & \text{when the flow is from } P_0 \text{ to } P_j \\ \phi_{P_j}, & \text{when the flow is from } P_j \text{ to } P_0 \end{cases} \quad (3.12)$$

First order, second order mixing method

$$\phi_j^* = \phi_j^{FO} + \gamma_\phi (\phi_j^{SO} - \phi_j^{FO}) \quad (3.13)$$

Here, ϕ^{FO} represents the value of a first order approximation and ϕ^{SO} represents the value of a second order approximation. The primary and secondary mixing methods are primary windward when the value of parameter γ is 0. When this value is 1, the mixing methods are a secondary central difference.

3.3.3 Diffusion Terms

Flux on the cell surface due to diffusion of variable ϕ is approximated by the following equation.

$$D_j = \int_{S_j} \Gamma_\phi \mathit{grad}\phi \cdot ds \approx \Gamma_{\phi,j} (\mathit{grad}\phi)_j^* \cdot s_j \quad (3.14)$$

Here, Γ_ϕ is a diffusion coefficient on the cell surface. The value $(\mathit{grad}\phi)_j^*$ of the cell interface is found as shown below.

$$(\mathit{grad}\phi)_j^* = (\mathit{grad}\phi)_j + \left(\frac{\phi_{P_j} - \phi_{P_0}}{|d_j|} - \frac{\overline{\mathit{grad}\phi \cdot d_j}}{|d_j|} \right) \frac{|d_j|s_j}{d_j \cdot s_j} \quad (3.15)$$

Here, $(\mathit{grad}\phi)$ is a value found using equation (4.7) and $\overline{\mathit{grad}\phi}$ is an arithmetical mean of the center of an adjacent cell. The CCFD uses a collocated grid method that arranges variables in the cell center. Because of this, numerical vibrations will occur in pressure and velocity when using values to a simple arithmetical mean is applied while calculating values at the cell interface. Thereupon, numerical vibrations are controlled by giving a quadratic term to the diffusion term as shown in equation (4.15).¹⁾

3.3.4 Source Terms

The source acting on cubic volume such as acceleration of gravity during heat generation or at the location of flow while performing heat transfer analysis and the source acting on surfaces such as heat flux acting on the surface of a physical object is approximated as shown below.

Surface source

$$Q_{\phi S} = \int_S q_{\phi S} \cdot ds \approx$$

$$\begin{cases} \sum_{j=1}^{n_f} \left(\left[\mu_{eff} (\mathbf{grad} \mathbf{v})^T - \left(\frac{2}{3} \mu_{eff} \mathbf{div} \mathbf{v} + p \right) \mathbf{I} \right]_j \cdot \mathbf{i}_i \right) \cdot s_j & , \text{for } \phi = v_i \\ 0 & , \text{for } \phi = c_i, e, k, \varepsilon \end{cases} \quad (3.16)$$

Cubic volume source

$$Q_{\phi V} = \int_V q_{\phi V} dV \approx (q_{\phi V})_{P_0} V_{P_0} \quad (3.17)$$

3.3.5 Boundary Conditions

Although advective terms and diffusion terms are evaluated on the surface of the cell, boundary conditions at the boundary of a target region are assigned. The conditions assigned to a boundary are broadly divided into Dirichlet type boundary conditions and Neumann type boundary conditions.

Dirichlet type boundary conditions

ϕ_j^* of equation (3.10) of the advective term is calculated by the already known value ϕ_B of the boundary. In addition, ϕ_{P_j} of equation (3.15) of the diffusion term is also replaced with already known value ϕ_B of the boundary and calculated.

Neumann type boundary conditions

This type of boundary conditions can be calculated by replacing the gradient of a dependent variable for a diffusion term with the boundary condition.

Details of other conditions will be described later.

3.3.6 Algebraic Equations

By means of using equations (3.2) to (3.17), equation (2.1) arrives back at the linear simultaneous equation shown below using the value of ϕ at the center of the cell the value of the adjacent cell.

$$a_{\phi_0} \phi_{P_0} - \sum_{j=1}^{n_f} a_{\phi_j} \phi_{P_j} = b_{\phi} \quad (3.18)$$

Here, each term is calculated as shown below.

$$a_{\phi_j} = \Gamma_{\phi_j} \frac{s_j \cdot s_j}{d_j \cdot s_j} - \min(\dot{m}_j, 0)$$

$$a_{\phi_0} = \sum_{j=1}^{n_f} a_{\phi_j} + \frac{(\rho V)_{P_0}^{m-1}}{\delta t_m}$$

$$\begin{aligned}
b_\phi &= \sum_{j=1}^{n_f} \Gamma_{\phi_j} \left((\text{grad}\phi)_j \cdot s_j - \overline{\text{grad}\phi} \cdot d_j \frac{s_j \cdot s_j}{d_j \cdot s_j} \right) \\
&\quad - \sum_{j=1}^{n_f} \frac{\gamma_\phi}{2} \dot{m}_j \left((r_j - r_{P_0}) \cdot (\text{grad}\phi)_{P_0} + (r_j - r_{P_j}) \cdot (\text{grad}\phi)_{P_j} + (\phi_{P_j} - \phi_{P_0}) \text{sgn}(\dot{m}_j) \right) \\
&\quad + Q_{\phi_s} + Q_{\phi_v} + \sum_{B=1}^{n_B} a_{\phi_B} \phi_B + \frac{(\rho V \phi)_{P_0}^{m-1}}{\delta t_m}
\end{aligned}$$

Here, $n_B = n_f - n_i$ is the number of boundaries.

3.3.7 Pressure Compensation Calculations

The velocity obtained by solving equation (3.18) does not always satisfy the law of conservation of mass. Therefore, a pressure must be compensated so as to satisfy the law of conservation of mass and the velocity must also be compensated at the compensated pressure. The CCFD uses a SIMPLE type algorithm to compensate the pressure and velocity. In order to control pressure oscillations due to using a collocated grid during compensation, we use a technique to calculate the velocity and density at the cell surface.

Calculations of velocity at the cell surface use the following equation.

$$v_j^* = v_j - \left(\frac{\overline{V_{P_0}}}{a_{v_0}} \right) \left\{ \frac{p_{P_j} - p_{P_0}}{|d_j|} - \frac{\overline{\text{grad}p}}{|d_j|} \right\} \frac{|d_j| s_j}{d_j \cdot s_j} \quad (3.19)$$

Here, the first term on the right side of equation (3.19) is the velocity calculated by equation (2.7) and the second term is a term for controlling pressure oscillations due to the collocated grid.

The density when calculating the mass flux is calculated using the following equation.

$$\rho_j^* = \rho_j^{UD} + \gamma_\rho (\rho_j^{CD} - \rho_j^{UD}) \quad (3.20)$$

Here, γ_ρ uses 0.9 to 0.95 as parameters for stabilization.

$$\frac{(\rho V)_{P_0} - (\rho V)_{P_0}^{m-1}}{\delta t_m} + \sum_{j=1}^{n_f} \dot{m}_j = 0 \quad (3.21)$$

A linear simultaneous equation is derived for the pressure compensation shown below.

$$a_{P_0'} p_{P_0}' - \sum_{j=1}^{n_f} a_{P_j'} p_{P_j}' = b_{p'} \quad (3.22)$$

Each term within equation (3.22) is calculated as shown below.

$$a_{P_j'} = \rho_j^* \left(\frac{\overline{V_{P_0}}}{a_{v_0}} \right) \frac{s_j \cdot s_j}{d_j \cdot s_j} - \left[(1 - \gamma_\rho) \min(v_j^* \cdot s_j, 0) + \frac{1}{2} \gamma_\rho v_j^* \cdot s_j \right] \left[\left(\frac{\partial p}{\partial p} \right)_{P_j} \right] \beta_p$$

$$a_{p_0} = \sum_{j=1}^{n_f} \check{\alpha}_{p'_j} + \frac{V_{P_0}}{\delta t_m} \left(\frac{\partial \rho}{\partial p} \right)_{P_0}$$

$$b_{p'} = -\sum_{j=1}^{n_f} \dot{m}_j - (\rho V)_{P_0} - (\rho V)_{P_0}^{m-1}$$

Here, $\check{\alpha}_{p'_j}$ is the conjugate portion of $a_{p'_j}$.

The velocity, pressure, density, and mass flux are corrected using the compensation value of the pressure calculated from equation (3.22) as shown below.

$$v_{P_0} = v_{P_0,pred} + v'_{P_0} = v_{P_0,pred} - \frac{1}{a_{v_0}} \sum_{j=1}^{n_f} p'_j s_j \quad (3.23)$$

$$p_{P_0} = p_{P_0,pred} + \beta_p p'_{P_0} \quad (3.24)$$

$$\rho_{P_0} = \rho_{P_0,pred} + \left(\frac{\partial \rho}{\partial p} \right) \beta_p p'_{P_0} \quad (3.25)$$

$$\dot{m}_j = \dot{m}_{j,pred} + \dot{m}' = \dot{m}_{j,pred} - a_{p'_j} p'_{P_0} + \check{\alpha}_{p'_j} p'_{P_0} \quad (3.26)$$

Here, β is a coefficient to stabilize the calculation and uses 0.2 to 0.3.

Boundary conditions

The boundary conditions of a Poisson equation for pressure compensation are dependent on the boundary conditions of the law of conservation of momentum. Boundary conditions of gradient 0 are assigned for the pressure compensation at a boundary where the flow rate is fixed. In addition, Dirichlet boundary conditions are assigned to pressure compensation for the boundary conditions of a fixed pressure.

3.4. Algorithms

The law of conservation of flow rate and temperature are returned to the form of equation (3.18). Although this is the case, since there is non-linearity for the momentum equation, the solution must be calculated by repeating the linearized equation and then performing a convergent calculation. Also, since each of the dependent variables are not independent from each other, each variable must be linked and solved. Hereupon, an enormous amount of memory and calculation time are required to consider the relation of each of the dependent variables once time and then solve. Because of this, a method is used that finds solutions so as to satisfy each relevance by individually solving each of the dependent variables and then performing repeated calculations.

CCFD supports SIMPLE algorithm, which is effective for solving steady state flow, and SMAC algorithm for unsteady calculations.

3.4.1 SIMPLE algorithm

SIMPLE algorithm uses the procedure shown below.

1. Uses an already known value to form and linearize coefficient matrix a_{ϕ_j} and source term b_{ϕ} for equation (3.18).

As shown below, the linear simultaneous equation of this result is derived.

$$A_{\phi} \phi = b_{\phi} \quad (3.27)$$

Here, A_ϕ is a matrix of $N \times N$. Vector ϕ is a dependent variable vector in the center of N number of cells and b_ϕ is a source vector. Matrix A_ϕ has the following characteristics.

- Irregular symmetrical sparse matrix. Has non-zero terms of number of cells + 1 adjacent to the target cell in each matrix.
 - Has superdiagonal angle of $a_{\phi_0} \geq \sum_{j=1}^{n_i} a_{\phi_j}$.
2. Solves equation (3.27) for each dependent variable. Because each coefficient matrix and the right side are approximated using the previous step value at this time, solving this equation is not strictly required.
 3. Repeats until steps 1 and 2 are a predetermined convergence error.

The CCFD solves equation (3.27) using and AMG (Algebraic Multi grid) method from the above characteristics.

The flow of the entire calculation is summarized as follows.

1. Set initial values of dependent variables
2. Update articulation points in time $t_m + \delta t_m$ and calculate volume change δV_j
3. Calculate the flow rate in each direction using equation (3.27)
4. Calculate the pressure compensation value using equation (3.27)
5. Calculate the turbulent kinetic energy using equation (3.27)
6. Calculate the Magnussen velocity using equation (3.27)
7. Calculate the temperature using equation (3.27)
8. Calculate the scalar variables using equation (3.27)
9. Repeat Steps 3 to 8 until reaching a predetermined number of sweeps
10. Repeat Steps 2 to 9 until reaching a predetermined time

The action from Step 3 to Step 9 is a repetition of a SIMPLE method and the action from Step 2 to Step 9 is a repetition of an unsteady calculation.

3.4.2 Under-relaxation

If equation (3.27) is repeatedly calculated, variations in the values will increase rapidly often making it impossible to perform stable calculations. Because of this, the CCFD transforms the coefficient matrix and right side vector of equation (3.27) as shown below and then lessens variations in the values and performs the calculation using a reiteration calculation process.

$$A_\phi \Rightarrow A_\phi + \frac{1 - \beta_\phi}{\beta_\phi} D_\phi, b_\phi \Rightarrow b_\phi + \frac{1 - \beta_\phi}{\beta_\phi} D_\phi \phi^{k-1} \quad (3.28)$$

Where, β_ϕ is a relaxation coefficient and is a value between 0 to 1. D_ϕ is an diagonal term of matrix A_ϕ and ϕ^{k-1} is a value before one step of the reiteration process.

3.4.3 SMAC algorithm

Because the first term of the equation (3.18) can be transformed into a following expression,

$$a_{\phi_0} \phi_{P_0} = \phi_{P_0}^{m-1} \sum_{j=1}^{n_f} a_{\phi_j} + \phi_{P_0}^m \frac{(\rho V)_{P_0}^{m-1}}{\delta t_m} \quad (3.29)$$

an equation as follows is derived from the equation (3.18).

$$\phi_{P_0}^m = \frac{\delta t_m \left(\sum_{j=1}^{n_f} a_{\phi_j} \phi_{P_j}^{m-1} - \phi_{P_0}^{m-1} \sum_{j=1}^{n_f} a_{\phi_j} + b_\phi \right)}{(\rho V)_{P_0}^{m-1}} \quad (3.30)$$

If dependent variable in equation (3.30) means fluid velocity, fluid velocity is able to calculate explicitly. However, fluid velocity calculated by equation (3.30) does not satisfy the equation of continuity (2.1). Therefore, fluid velocity and pressure are corrected by using the equations (3.23) . (3.26). Note that β in those equations is 1.0 for SMAC algorithm. Furthermore, relaxation of the coefficient matrices and right hand side vectors will not performed in the case of SMAC algorithm.

3.5. Boundary Conditions

3.5.1 Wall Conditions

Three conditions; slip, non-slip, and wall function are most often assigned as conditions when a fluid makes contact with a solid wall. The CCFD can take these three types of boundary conditions into consideration.

slip condition

The slip condition is represented by the following equation.

$$u_n = 0, \frac{\partial u_t}{\partial n} = 0 \quad (3.29)$$

Here, u_n is a vertical velocity component with respect to the wall and u_t is a parallel velocity component.

non-slip condition

The non-slip condition is represented by the following equation.

$$u_n = 0, u_t = 0 \quad (3.30)$$

Wall function

The non-slip condition normally represented by equation (3.30) is assigned to locations where fluid makes contact with a wall. However, when there is a turbulent state with a large number of Re, calculations must be performed using very fine lattices in order to simulate the boundary conditions in a non-slip condition. The CCFD considers boundary conditions close to a wall by providing a velocity close to a wall using a wall function of the following logarithmic law.

$$\mu_w = \frac{y^+}{u^+} \mu \quad (3.31)$$

Here, the following equation is true.

$$u^+ = \begin{cases} y^+ & , y^+ < y_v^+ \\ \frac{1}{K} \ln(\epsilon y^+) & y^+ \geq y_v^+ \end{cases} \quad (3.32)$$

K is a Larman constant and ϵ is a constant dependent on the surface roughness of the wall. y^+ is the non-dimensional distance from the wall.

The following equation is true for a 0 equation model.

$$y^+ = \frac{1}{K} \frac{\mu_t + \mu}{\mu} \quad (3.33)$$

The following equation is true for other models.

$$y^+ = \frac{\rho C_\mu^{1/4} k_{P_0}^{1/2} \delta n_{P_0}}{\mu} \quad (3.34)$$

Here, μ is a coefficient of molecular viscosity and μ_t is an eddy viscosity coefficient. C_μ is an turbulent model coefficient. k is turbulent kinetic energy, δn is the distance from the wall, and P_0 is the center of the cell making contact with the wall.

The viscosity low wall thickness y_v^+ is represented by the following equation.

$$y_v^+ = \frac{1}{K} \ln(\epsilon y_v^+) \quad (3.35)$$

3.5.2 Natural Outflow

The condition below is considered to be an outflow condition from the target calculation region.

$$p_w = 0 \quad (3.36)$$

Here, p_w is the pressure at the outflow surface of the cell thought to be a free flowing outflow.

Mass flux is calculated so as to satisfy successive equations at a boundary when there are incompressible fluids due to assigning the conditions of equation (3.36). Various states can be considered for conditions related to energy and chemical species by separately assigning a Dirichlet condition or a Neumann condition.

3.5.3 Inflow Conditions

Inflow conditions of fluid towards the target calculation region are considered by providing the velocity at the surface of the cell. The CCFD calculates the mass flux based on a fixed flow rate and reflects this in the law of conservation of mass and the law of conservation of momentum.

3.5.4 Temperature Boundary (chemical species)

The CCFD considers the following condition as a boundary condition of temperature (chemical species).

Heat generation

Heat generation (source) can be considered by providing s_{h_i} of equation (2.1) of the law of conservation of energy.

Heat convection (inhomogeneous Neumann conditions)

Allows inhomogeneous Neumann boundary conditions to be set.

Heat flux

Heat flux of the surface of the cell can be provided.

Fixed temperature

The temperature of the cell can be directly set.

End