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Analysis of Heat Transfer Problems by a Consistent Formulation of the Energy Equation

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1. Introduction

After the SIMPLE algorithm was introduced in the area of computational fluid dynamics (CFD) by Patankar [1], many thermal hydraulic analysis codes based on this algorithm have been developed commercially or for research purposes. The main features of the algorithm are easy to modify and easy to implement numerical or physical models in it by the nature of its segregated and iterative method to satisfy the conservation laws. The numerical method can be applicable to geometrically and physically complex problems. One of the problems is a gas mixture flow coupled with heat transfer in a region including a solid structure. For this kind of conjugate heat transfer problem, the energy equation is usually decoupled and solved sequentially in fluid and solid regions because there is a jump in the enthalpy at the solid-fluid interface. At the interface, the enthalpy is double-valued, but the temperature is continuous. If the energy equation with temperature as a primary dependent variable is used, the heat transfer can be solved in a directly coupled manner. Murthy and Mathur [2] introduced a form of the energy equation whose primary dependent variable is temperature. The main idea was to add unsteady and convection terms expressed with temperature and to solve the equation by the iterative method. The method is useful for the conjugate heat transfer problems because the discretized equation is expressed with temperature. Similar to this method, a new method is derived in this study, which is a consistent formulation of the energy equation for a heat transfer in a solid, liquid and gas mixture. The enthalpy form of the energy equation is used in the method. But the final discrete form of the equation is expressed with temperature. This discretization is based on a dual-time delta formulation.

2. Numerical Method

In this study, the compressible Reynolds-averaged Navier-Stokes equations is used. All the governing equations can be cast into the following integral form:

$$\frac{\partial}{\partial t}\int \rho\phi\, dV + \int \rho\phi \vec{v}\, d\vec{S} - \int \Gamma \nabla\phi\, d\vec{S} = \int q_\phi\, dV \qquad (1)$$

Where ρ is a density of the fluid, ϕ is the dependent variable of the transport equation, $\vec{v}$ is a velocity vector, Γ is a diffusion coefficient, for example, $\Gamma = \mu$ for the momentum equation. q_ϕ is a source term of the equation.

By the context of the dual-time delta formulation, the transport equation can be written as:

$$\left[\frac{3\rho_i V}{2\Delta t} + \frac{\rho_i V_i}{\Delta\tau} + A_{\phi i}\right]\Delta\phi_i^{n+1,m} + \sum_j A_{\phi j}\Delta\phi_j^{n+1,m} = q_\phi^{n+1,m}V_i - \sum_f (C_f^{n+1,m} - D_f^{n+1,m})S_f - \frac{\rho_i V}{2\Delta t}\left(3\phi^{n+1,m} - 4\phi^n + \phi^{n-1}\right) \qquad (2)$$

In this formulation, a pseudo-time term is added to remedy the errors from the linearization of the equation, which is similar to a term in the iterative under-relaxation formulation. A second order backward differencing is used for the physical time derivative (Δt), and the Euler implicit differencing is employed for the pseudo-time derivative ($\Delta\tau$). In this study, a second-order upwind or central differencing scheme is used for the convective flux and a second-order central scheme is used for the diffusive flux on the right hand side.

Generally, the pressure gradient term included in the momentum equation is not known priory. With the approximate solution of a pressure field, the velocity calculated from the momentum equation is not correct. So it is necessary to correct the velocity in order for a mass conservation. The equation for the mass correction is derived by using the SIMPLEC algorithm.

3. Energy Equation Discretization

In order to describe the energy conservation law in a flow field, many forms of energy equations exist. In this study, static enthalpy equation is used because it has advantages in numerical and physical point of view.

$$\frac{\partial}{\partial t}\int \rho h\, dV + \int \rho h \vec{v}\cdot d\vec{S} = \int \vec{q}_h \cdot d\vec{S} + \int s_h\, dV + \int \mathbf{T} : \nabla\vec{v}\, dV + \int \vec{v}\cdot\nabla p\, dV + \frac{\partial}{\partial t}\int p\, dV \qquad (3)$$

In eq. (3), h is static enthalpy. For a multi-species flow with a chemical reaction, it becomes static thermo-chemical enthalpy which contains the enthalpy of formations of the species. In the case of the high speed flow, h becomes total enthalpy with a modified work term in eq. (3). The SIMPLE algorithm requires that the energy equation be discretized in a implicit form. But, a problem is encountered in discretizing the energy equation because of the inconsistency of the convection and conduction terms of the equation. Usually, temperature of the conduction term is changed to enthalpy and the discrete energy equation is expressed in terms of enthalpy. But it is not desirable for conjugate heat transfer problems where the enthalpy is not continuous on the interface of the solid and fluid. In this study, a new formulation is proposed to discretize the energy equation with temperature as a primary variable.

In order to linearize the enthalpy equation in terms of the temperature, the pseudo-time term of the static

enthalpy on a fixed grid is added into the energy euqation.

$$\int \rho \frac{\partial h}{\partial \tau} dV + \frac{\partial}{\partial t}\int (\rho h - p)\, dV + \int \rho h \vec{v} \cdot d\vec{S} = \int \vec{q}_h \cdot d\vec{S} + \int s_h \, dV + \int \mathbf{T} : \nabla \vec{v}\, dV + \int \vec{v} \cdot \nabla p \, dV \quad (4)$$

The Pseudo-time term is changed to a temperature derivative by the chain rule.

$$\int \rho \frac{\partial h}{\partial \tau} dV = \rho V \frac{\partial h}{\partial \tau} = \rho V \frac{\partial h}{\partial T}\frac{\partial T}{\partial \tau} = \rho V C_p \frac{\partial T}{\partial \tau} \quad (5)$$

The surface integral of the enthalpy convection is discretized to summation of the enthalpy flux on each face of a cell.

$$\int \rho h \vec{v} \cdot d\vec{S} = \sum_f C_f S_f \quad (6)$$

The convective flux on each face f can be written as $C_f = J_f H_f$, where J_f is a mass flux on the face.

For an implicit scheme, the convective flux is linearized, where the mass flux is frozen.

$$C_f^{m+1} = C_f^m + \left(\frac{\partial C}{\partial T}\right)_f \Delta T = (J_f h_f)^m + J_f \left(\frac{\partial h}{\partial T}\right)_f \Delta T = (J_f h_f)^m + J_f C_p \Delta T \quad (7)$$

The temperature derivative of the enthalpy contains only the specific heat because the mechanical energy (in the case of total enthalpy) and chemical enthalpy of formations are not directly dependent on temperature.

The thermal diffusion can be discretized as:

$$\int k_{eff} \nabla T \cdot d\vec{S} = \sum_f D_f S_f \quad (8)$$

And the diffusion flux on each face is departed into primary and secondary diffusion fluxes.

$$D_f = \frac{k_{eff}}{ds \cdot \hat{n}}(T_{cj} - T_{c0}) + k_{eff}\left[\overline{\nabla T}_f \cdot \hat{n} - \left(\overline{\nabla T}_f \cdot \hat{ds}\right)\frac{1}{ds \cdot \hat{n}}\right] \quad (9)$$

The diffusion flux can be linearized as:

$$D_f^{m+1} = D_f^m + \frac{dD_f}{dT}\Delta T^m = D_f^m + \left(\frac{dD_f}{dT}\right)_{c0}\Delta T_{c0}^m + \left(\frac{dD_f}{dT}\right)_{cj}\Delta T_{cj}^m$$

Because the primary diffusion flux is more important and larger than the secondary diffusion flux, only the primary term which is expressed in terms of temperature is linearized.

$$\left(\frac{dD_f}{dT}\right)_{c0} = -\frac{k_{eff}}{ds \cdot \hat{n}}, \quad \left(\frac{dD_f}{dT}\right)_{cj} = \frac{k_{eff}}{ds \cdot \hat{n}} \quad (10)$$

The unsteady term of the energy equation contains enthalpy and pressure, which can be changed to thermo-chemical energy for the enthalpy form of the energy equation.

$$\frac{\partial}{\partial t}\int (\rho h - p) dV = \frac{\partial}{\partial t}\int \rho e \, dV \quad (11)$$

The unsteady term is discretized by three-time level Euler implicit method.

$$\frac{\partial}{\partial t}\int \rho e \, dV = \frac{V}{2\Delta t}\left[3\Delta(\rho e)^{n+1,m} + 3(\rho e)^{n+1,m} - 4(\rho e)^n + (\rho e)^{n-1}\right] \quad (12)$$

The first term of the discretized right hand-side of the equation is added in the implicit part and the other terms are added in the explicit part of the discretized energy equation.

In order to add the first term expressed in the total energy or internal energy into the implicit part of the discretized energy equation in terms of the temperature, it is necessary to linearize it to the temperature direivative term by a chain rule.

$$\Delta(\rho e) = \frac{\partial(\rho e)}{\partial T}\Delta T \approx \rho(C_{p,m} - R)\Delta T \quad (13)$$

By summing all the terms, the discretized energy equation with explicit temperature variable can be obtained.

$$\left[\frac{3\rho V(C_p - R)}{2\Delta t} + \frac{\rho V C_p}{\Delta \tau} + A_\phi\right]\Delta T_{c0}^{n+1,m} + \sum_{cj} A_{\phi,cj}\Delta T_{cj}^{n+1,m} = q_{\phi,c0}^{n+1,m} V_{c0} - \sum_f (C_f^{n+1,m} - D_f^{n+1,m}) S_f - \frac{V}{2\Delta t}\left[3(\rho E)^{n+1,m} - 4(\rho E)^n + (\rho E)^{n-1}\right]_{c0} \quad (14)$$

4. Numerical Results

The numerical method proposed in this study was validated by solving a conjugate natural convection in a cavity. Fig. 1 shows the schematic of the problem and the temperature contours, which are continuous at the solid-fluid interface.

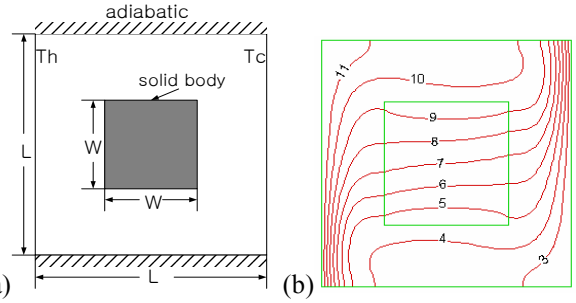

Fig. 1 Natural convection in a cavity with centered solid body (a) schematic, (b) temperature contours

5. Conclusion

In this study, a new formulation of an energy equation with temperature as a primary dependent variable was introduced. It can be applicable to most of heat transfer problems consistently including conjugate heat transfer in a gas mixture and solid region.

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