Computational Method for Thermal Interactions between Compressible Fluids and Complicated-Shaped Structures with Multiphase Modeling

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Abstract

In this paper, a new computational method based on multiphase model was presented to deal with the thermal interactions between compressible fluids and complicated-shaped structures with thermal conductivities as well as its mechanical interactions. The numerical procedures of our method are divided into three stages, advection, diffusion and acoustic stages, and the phase averaged governing equations are discretized with a finite volume method (FVM). The present method was applied to the natural convection flows in a rectangular cavity and the calculated results were compared with the reference computational results for temperature and velocity distributions. As a result, it was shown that the natural convection flows could be reasonably simulated by our method. In addition, the natural convections arising in the porous media were calculated with the present method. Through the numerical experiments, its applicability to complicated-shaped structures was discussed.

Keywords: Compressible fluid, Complicated-shaped structure, Multiphase model, Natural convection.

Introduction

In many engineering subjects, it is important to predict accurately heat transfers in the domain, which contains compressible fluids and complicated-shaped structures. In the management of spent fuel storage system of nuclear power plants with the concrete cask for extended periods, the temperature distributions in the canister, which stores spent fuels and helium gas, need to be predicted accurately for the development of the helium leak detection system (Takeda et al., 2008). The canister has complicated-shaped internal structures and the temperature and pressure differences are large when the helium leakage from the canister occurs. Thus, it is essential to estimate the thermal interactions compressible helium gas and the influence of internal structures.

For example, a finite element method (FEM) using unstructured grids has been used with thermal coupled problem between fluids and complex geometries (Goung et al., 1990). Such methods using unstructured grids can accurately predict the phenomena. However, the generations of grids become difficult as the shapes of geometries become complex.

The multiphase model (Ushijima et al., 2007 and 2009) enables us to predict thermal and mechanical interactions between incompressible fluids and complicated-shaped structures easily with simple structured grids. In this paper, a new computational method based on multiphase model was proposed to deal with the interactions between compressible fluids and complicated-shaped structures. The present method was applied to the natural convection flows in a rectangular cavity. As a result, it was shown that the natural convection flows could be reasonably simulated by our method. In addition, the natural convections arising in the porous media were calculated with the present method. Through the numerical experiment, its applicability to complicated-shaped structures was discussed.

Computational Method

Governing Equations

The multiphase field consisting of fluids and solids is considered, where fluids are compressible and each phase is immiscible. In this study, solids are taken as fluids which do not move.

Averaged governing equations for the multiphase field, which contain compressible fluids, consist of mass conservation equation in Eulerian description, momentum equations and energy equation given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i \quad (2)$$

$$\frac{\partial (\rho e)}{\partial t} + \frac{\partial (\rho e u_j)}{\partial x_j} = -p \frac{\partial u_i}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j} \quad (3)$$

where *t* is time, x_i is the *i*-th component of two-dimensional orthogonal coordinates and g_i is the acceleration of external force in x_i direction. While velocity component u_i and internal energy *e* are the mass-averaged value in the mixture of phases, volume-averaged variables are defined for density ρ , pressure *p*, viscous stress τ_{ij} , heat flux q_j . For example, *e* and *p* are defined as

$$e = \frac{\sum_{k} \rho_{k} V_{k} e_{k}}{\sum_{k} \rho_{k} V_{k}} \quad \text{and} \quad p = \frac{\sum_{k} V_{k} p_{k}}{V} \quad (4)$$

Furthermore, e, τ_{ij} , q_j and the state equation are given by

$$e = C_V T \quad (5)$$

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_m}{\partial x_m} \delta_{ij} \quad (6)$$

$$q_j = -\lambda \frac{\partial T}{\partial x_j} \quad (7)$$

$$p = (\gamma - 1)\rho e \quad (8)$$

where C_V , T, μ , λ and γ are specific heat at constant volume, temperature, viscosity, thermal conductivity and specific heat ratio respectively. These are volume-averaged variables and coefficients same as ρ , p, τ_{ij} and q_j .

Numerical Procedures

In our method, the numerical procedures are divided into three stages, advection, diffusion and acoustic stages, like CCUP (Yabe et al., 2004) and TCUP method (Himeno et al., 2003). The governing equations are written by conservation forms and the multiphase model is applied. The governing equations of each stage are discretized with a finite volume method (FVM) and variables, ρ , \boldsymbol{u} , T and p, are updated in all stages. Thus, the mass conservation law is sufficiently satisfied in a calculation area. On the other hand, in CCUP and TCUP method, the governing equations are written by non-conservation forms. Therefore, the conservation of mass in the calculation area is not necessarily satisfied.

Figure 1 shows the flow chart of numerical procedures. In the advection and diffusion stages, advection and diffusion terms are calculated respectively. Pressure and gravity terms are calculated in the acoustic stage. After that, phase averaged variables are updated based on volume of solids. These calculations are performed iteratively and numerical solutions are calculated in time evolution. In what follows, variables after advection and diffusion stages will be expressed as Q' and Q'' respectively. In addition, variables after acoustic stage are Q^{n+1} .



Figure 1. Flow chart of numerical procedures

Advection Stage

Governing equations of advection stage are given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \quad (9)$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = 0 \quad (10)$$

$$\frac{\partial (\rho e)}{\partial t} + \frac{\partial (\rho e u_j)}{\partial x_i} = 0 \quad (11)$$

Equations (9), (10) and (11) express advection equations of ρ , ρu , ρe respectively. The advection terms are calculated with a fifth-order TVD scheme (Harten, 1984). After that, *T*' and *p*' are updated from ρ ', *u*', *e*' with Eqs.(5) and (8).

Diffusion Stage

Governing equations of diffusion stage are indicated as follows :

$$\frac{\partial \rho}{\partial t} = 0 \quad (12)$$
$$\frac{\partial (\rho u_i)}{\partial t} = \frac{\partial \tau_{ij}}{\partial x_j} \quad (13)$$
$$\frac{\partial (\rho e)}{\partial t} = \tau_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j} \quad (14)$$

In this stage, right-hand sides of Eqs.(13) and (14) are calculated and variables are updated with the following equations :

$$\rho^{"} \frac{u_{i}^{"} - u_{i}^{'}}{\Delta t} = \frac{\partial \tau_{ij}^{'}}{\partial x_{j}} \quad (15)$$

$$\frac{\rho^{"} C_{P} (T^{"} - T^{"})}{\gamma \Delta t} = -\frac{\partial (\rho^{'} C_{V} T^{'} u_{j}^{'})}{\partial x_{j}} + \frac{\partial (\tau_{ij}^{'} u_{j}^{'})}{\partial x_{j}} - \frac{\partial q_{j}^{'}}{\partial x_{j}} - \frac{\rho^{'}}{2} \frac{\partial u_{j}^{'}}{\partial t} \quad (16)$$

$$p^{"} - p^{'} = \frac{\gamma - 1}{\gamma} \frac{\rho^{"} C_{P}}{\rho^{"} C_{P} \mu_{J} + 1} (T^{"} - T^{'}) \quad (17)$$

where μ_J is Joule-Thomson coefficient.

Acoustic Stage

Governing equations of acoustic stage are given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \quad (18)$$
$$\frac{\partial (\rho u_i)}{\partial t} = -\frac{\partial p}{\partial x_i} + \rho g_i \quad (19)$$
$$\frac{\partial (\rho e)}{\partial t} = -p \frac{\partial u_i}{\partial x_i} \quad (20)$$

Equations (18), (19) and (8) applied to Eq.(20), we can obtain the equation of p^{n+1} as follows :

$$\frac{1}{\rho''C_s^2}\frac{p^{n+1}-p''}{\Delta t} = -\frac{\partial}{\partial x_i} \left(-\frac{1}{\rho''}\frac{\partial p^{n+1}}{\partial x_i}\Delta t + u_i''\right) \quad (21)$$

where C_s is the sound speed. Equation (21) is discretized and solved with the SOR method (Young, 1954). The variables, u^{n+1} , e^{n+1} and ρ^{n+1} , are calculated with the following equations :

$$u_{i}^{n+1} = u_{i}'' + \left(-\frac{1}{\rho''}\frac{\partial p^{n+1}}{\partial x_{i}} + g_{i}\right)\Delta t \quad (22)$$

$$\rho''\frac{e^{n+1} - e''}{\Delta t} = p^{n+1}\frac{\partial u_{i}^{n+1}}{\partial x_{i}} \quad (23)$$

$$\frac{\rho^{n+1} - \rho^{n}}{\Delta t} = -\frac{\partial \rho^{n}u_{i}^{n+1}}{\partial x_{i}} \quad (24)$$

Application

Natural Convection in a Rectangular Cavity

In order to confirm the validity of the present method, it was applied to the 2D natural convection flows in a rectangular cavity as shown in Fig.2. The lengths l_1 and l_2 are 0.04 [m], while the left-hand side wall is heated at T_h and the right-hand side wall is cooled at T_c , the temperature difference $\Delta T = T_h - T_c$ is 1.465 [K] in Fig.2. Adiabatic conditions are imposed on the top and bottom walls. On the wall boundaries, non-slip conditions are imposed.

Fluids are taken as air, which satisfy the equation of state. The initial spatially averaged temperature T_0 and pressure P_0 are 283.15 [K] and 1.0 [atm]. Regarding physical properties of fluids, viscosity μ , thermal conductivity λ , specific heat at constant pressure and volume C_P , C_V , are $\mu = 1.82 \times 10^{-5}$ [kg/(m•s)], $\lambda = 2.587 \times 10^{-2}$ [W/(m•K)], $C_P = 1.007 \times 10^3$ [J/(kg•K)] and $C_V = 7.17 \times 10^2$ [J/(kg•K)] respectively. The number of fluid cells is 100×100 .

Figures 3, 4 and 5 show comparisons of calculated results in the steady states by the present method and reference results by TCUP method (Himeno et al., 2003). As shown in these figures, the predicted results are almost in good agreement with the results by TCUP method. From these results, it was shown that the present method enables us to predict a natural convection appropriately.

In addition, err^* , which made dimensionless the total change of the mass of air in a calculation area, is defined as $err^* = |M - M_0|/M_0$. Here M and M_0 are the total mass of air in the calculation area at each time step and in the initial state. The maximum value of err^* obtained in the calculation was 5.713×10^{-15} . From this result, it was shown that the mass conservation law is sufficiently satisfied in the calculation area.

In the following cases, the temperature difference was set to $\Delta T = 100$ [K] and density variations were compared with the result in $\Delta T = 1.465$ [K]. The density variations are estimated with Lagrangian derivative of non-dimensional density $D\rho^*/Dt$. Here ρ^* is given by $\rho^* = \rho / \rho_0$ and ρ_0 is the spatial averaged density in the initial state. It is noted that $D\rho^*/Dt = 0$ in incompressible fluids.

Figure 6 shows the distributions of $D\rho^*/Dt$ in the steady state and Table 1 shows maximum and minimum values of $D\rho^*/Dt$ in each case. In Figure 6 and Table1, the densities change near the heated and cooled wall and absolute values of variations increase as ΔT increases. In general, compressibility effects become large as ΔT increases. Thus, it can be said that calculated results are appropriate and the present method enable us to estimate the compressibility effects of fluids.





Figure 3. Comparison of temperature distributions (Left : present results, Right : TCUP (Himeno et al., 2003))

Figure 2. Calculation area







Figure 4. Comparison of u_1 distributionsFigure 5. Comparison of u_2 distributions(Left : present calculations, Right : TCUP (Himeno et al., 2003))



Table 1. Maximum and minimum values of $D\rho^*/Dt$

| $\Delta T[\mathbf{K}]$ | Max [1/s] | Min [1/s] |
|------------------------|------------------------|-------------------------|
| 1.465 | 1.615×10^{-3} | -1.618×10 ⁻³ |
| 100 | 1.576 | -1.663 |

Natural Convection in Porous Media with Thermal Conductivity

To confirm the applicability of the present method to complicated-shaped structures, natural convections in porous media with thermal conductivity were calculated.

As shown in Figure 7, 32 cylinders are located in a calculation area. The lengths l_1 and l_2 are 0.17 and 0.33 [m], while the diameter of the cylinders *d* is 0.03 [m] and the interval between each cylinder *s* is 0.01 [m] respectively. The left-hand side wall is heated at $T_h = 310$ [K] and the righthand side wall is cooled at $T_c = 300$ [K], the temperature difference $\Delta T = T_h - T_c$ is 10 [K] in Fig 7. Adiabatic conditions are imposed on the top and bottom walls. On the wall boundaries, non-slip conditions are imposed. The physical properties of fluids (air) were set same values as the preceding section and physical properties of the solids (cylinders) were same as that of fluids. In addition, the number of fluid cells is 51×99 .

Figure 8 shows temperature distributions ((a) t = 1.0 [s], (b) steady state). First, heats transferred by convections in the fluids area. After that, the temperatures of solids changed by heat conductions in the solids. Thus, the temperature differences between the fluids and the solids occurred at t = 1.0 [s] in Fig 8 (a). In the steady state, the temperatures of solids became equal to that of fluids as shown in Fig 8 (b). Figure 9 is the vertical distribution of T at $x_1^* = 0.5$ in the steady state. Here, x_i^* and T^* are defined as follows :

$$x_i^* = \frac{x_i}{l_i}$$
 and $T^* = \frac{T - T_m}{T_h - T_m}$ (25)

where, l_i is the length of the calculation area, T_h is the temperature of the heated wall and T_m is the temperature at $x_1^* = 0.5$ and $x_2^* = 0.5$. In the calculated result, the top area is high temperature and the bottom area is low temperature. This is the typical temperature distribution of the natural convection in the closed cavity.

Predicted the horizontal velocities u_1 at $x_1^* = 0.5$ and the vertical velocities u_2 at $x_2^* = 0.5$ are shown in Fig 10 and 11 respectively. Here, u_i^* is defined as follows :

$$u_i^* = \frac{u_i}{U_i} \qquad (26)$$

where, U_i is the maximum value of $|u_i|$ in the calculation area. As shown in these figures, buoyancydriven flows occurred near the heated and cooled walls and cyclic flows were predicted in the fluids area. Thus, it can be said that the present method enables us to predict the natural convections in porous media with thermal conductivity reasonably.



Figure 7. Calculation area

Figure 8. Temperature distributions



Figure 9. Vertical distribution of $T(x_1^* = 0.5)$



Conclusions

In this paper, a new computational method based on multiphase model was proposed to deal with the thermal and mechanical interactions between compressible fluids and complicated-shaped structures with thermal conductivities. The numerical procedures of our method are divided into three processes, advection, diffusion and acoustic stages, and the phase averaged governing equations are discretized with a finite volume method (FVM). Thus, the mass conservation law is sufficiently satisfied in a calculation area in our method.

The present method was applied to the natural convection flows in a rectangular cavity and the calculated results were compared with the reference computational results for temperature and velocity distributions. As a result, it was shown that the natural convection flows can be reasonably simulated by our method. It was also confirmed that the mass conservation law is satisfied sufficiently in the calculation area, and the present method enables us to estimate the compressibility effects of fluids by the temperature difference. In addition, the natural convections arising in the porous media were calculated with the present method. Through the numerical experiment, its applicability to complicated-shaped structures was verified.

References

- Young, D. M. (1954), Iterative Methods for Solving Partial Differential Equations of Elliptic Type, *Transactions of the American Mathematical Society*, Vol.76, pp.92-111.
- Harten, A. (1984), On a Class of High Resolution Total-Variation-Stable Finite-Difference Schemes, *SIAM Journal on Numerical Analysis*, Vol.21.
- Goung, J. L. and Soon H. C. (1990), Development of the finite element method of body fit nodalization for mixed convection analysis in rod bundles, *Nuclear Engineering and Design*, 122, pp.195-208.
- Yabe, T., Xiao, F. and Utsumi, T. (2001), The Constrained Interpolation profile Method for Multiphase Analysis. *Journal of Computational Physics*, 43, pp. 531-545.
- Himeno, T. and Watanabe, T. (2003), Thermo-Fluid Management under Low-Gravity Conditions (1st Report: TCUP Method for the Analysis of Thermo-Fluid Phenomena) (in Japanese), *Trans. JSME, Ser. B*, Vol.69, No.678, pp.266-273.
- Ushijima, S. (2007), Multiphase-model approach to predict arbitrarily-shaped objects moving in free surface flows. *Proc of APCOM'07-EPMESC XI*, MS41-3-1.
- Takeda, H., Wataru, K. Shirai, K. and Saegusa, T. (2008), Development of the detecting method of helium gas leak from canister. *Nuclear Engineering and Design*, Vol.238, pp.1220-1226.
- Ushijima, S. and Kuroda, N. (2009), Multiphase modeling to predict finite deformations of elastic objects in free surface flows. *Fluid Structure Interaction V, WIT Press*, pp.34-45.