Simulation of Thermophysical Flows

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Abstract: Recent progress of numerical methods for simulating flows coupled with thermophysical problems is overviewed and the development in our group is introduced. Our numerical method is based on the preconditioning method coupled with mathematical models of thermophysical properties. As typical numerical examples in which thermophysical properties are quite effective to the flow feature, results of natural convection of supercritical carbon dioxide across the critical point and that of water at approximately 4°C are briefly introduced.

1. Introduction

Computational fluid dynamics (CFD) may have been started from the study by Southwell (1940) in which a relaxation method for finite difference method (FDM) was proposed. From 1950s to 1980s, a number of compressible flow solvers have been proposed for simulating shock tube problems: approximate Riemann solvers, total variation diminishing (TVD), implicit methods, and so on. On the other hand, Harlow et al. (1965) presented a method for simulating free-surface flows in which Marker and Cell (MAC) method was proposed. This method is known as the origin of incompressible flow solvers based on the Poisson equation of pressure and the staggered grid.

Current CFD solvers can be divided mainly into such compressible flow solvers and incompressible flow solvers. Air flows are generally solved by the compressible flow solvers assuming an ideal gas. Water flows or low-speed air flows are solved by the incompressible flow solvers assuming that the density is constant.

The number of substances we know is beyond the number of atoms as shown in the table of elements. The state of substances changes to gas, liquid and solid according to pressure and temperature. Substances have their own thermophysical properties such as density, viscosity, heat conductivity, melting point, and boiling point. Even the density of liquid changes exactly. In addition, reactions may occur between different two substances. The difference of substances is crucial in material studies, but the difference has not always been important in fluid dynamics because of the singularity laws such as Reynolds number. Since thermophysical properties are almost constant or not changed drastically in a gas or liquid phase, flows can be solved approximately based on the singularity law. However, thermophysical values should be accurately evaluated, if phase change or reaction occurs in the flows.

In addition, substance becomes a supercritical fluid as increasing the pressure and temperature. It is known that supercritical fluids have anomalous properties especially near the critical point. Unfortunately current CFD approaches lack such consideration.

2. Preconditioning Method

Compressible flow solvers may be basically preferable if flows with the change of thermophysical properties are simulated. However, the solvers based on the time-marching method and the approximate Riemann solvers have a fatal problem, the so-called stiffness problem, if incompressible flows or very-slow flows are simulated by them. No convergence solution or none physical solution may be obtained. Turkel (1987) and Choi et al. (1993) proposed an approach combining incompressible and compressible flow solvers to avoid the stiffness: preconditioning method. A numerical speed of sound is introduced into a preconditioning matrix and compressible Navier-Stokes equations are multiplied by the matrix. The numerical speed of sound is changed smoothly between the physical value and a numerical value according to the flow velocity; the governing equations are changed between the compressible Navier-Stokes equations and pseudo-compressible Navier-Stokes equations. Weiss et al. (1995) proposed a preconditioning method for solving unsteady incompressible flows. Most of the preconditioning methods employ the approximate Riemann solvers which are employed for simulating compressible flows with shocks.

One of authors proposed a preconditioning method (Yamamoto, 2005-1) based on Roe's scheme (Roe, 1981) and LU-SGS scheme (Yoon et al., 1987). A new

preconditioned flux-vector splitting (PFVS) form was derived and the preconditioned Roe scheme and the preconditioned LU-SGS scheme were also derived using the PFVS form. The preconditioning methods can simulate not only transonic and supersonic flows with shocks but also vey-slow flows and natural convection. Finally we employ the preconditioning approach as the base method for simulating thermophysical flows.

3. Thermophysical Models

Substances have their own thermophysical properties. The values are changed according to the values of temperature and pressure. The phase is occasionally changed among gas, liquid, and solid. In addition, substances become supercritical fluids if the temperature and pressure are beyond the critical points. Figure 1 shows *p-T* phase diagram of carbon dioxide. If the values of pressure and temperature are beyond their values at the critical point, carbon dioxide becomes the supercritical fluid.

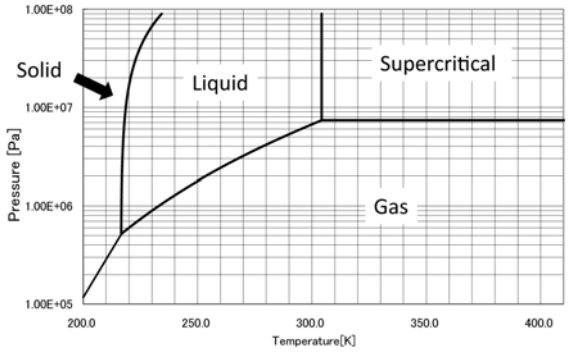


Figure 1 *p-T* phase diagram of carbon dioxide

Especially, supercritical fluids have anomalous properties near the critical point: maximum peak of isobaric specific heat and that of reaction rate; rapid change of solubility, zero surface tension, and so on. These anomalous properties are utilized for the decomposition of waste, the fabrication of nanoscale particles, heat exchangers, and so on, by chemical, material and mechanical engineers. Eckert et al. (1996) reviewed the research works of supercritical fluids in the *Nature*.

Ordinary CFD solvers employing the equation of state (EOS) for ideal gas cannot predict actual thermophysical values in flows of arbitrary substance. Fortunately, primary thermophysical properties such as density, viscosity and thermal conductivity have been mathematically modelled by chemical engineers for most of substances. For examples, we know several EOSs based on cubic-type and virial-type models. Cubic-type EOS is formed by a cubic equation based on the van der Waals EOS. The form is not so complicated as compared with that of virial-type EOS. Merkle et al. (1998) and Edward et al. (2000) applied their preconditioning methods coupled with a cubic EOS to the simulation of supercritical-fluid flows and gas-liquid two phase flows. We simulated thermal convection of supercritical carbon dioxide (Yamamoto 2005-2) using our preconditioning method coupled with Peng-Robinson EOS (P-R EOS) (1976) which is a modified EOS from the van der Waals EOS. The obtained results suggest that the solution is essentially different from ordinary solutions obtained by assuming an ideal gas. P-R EOS could be applied to the carbon dioxide reasonably. But, P-R EOS could not predict water accurately. It suggests that cubic-type EOS cannot be used as a general-purpose EOS for arbitrary substance.

On the other hand, virial-type EOS is formed by a polynomial equation. Even though the computational cost is relatively higher than that of cubic-type EOS, the accuracy is sufficiently preserved even if the temperature and pressure are changed between two phases. A virial-type EOS for carbon dioxide was standardized at IUPAC (1976). Figure 2 shows the density distributions while changing temperature at a different bulk pressure calculated from the EOS which can cover both supercritical and subcritical states. Density can be obtained continuously in all temperature and pressure conditions.

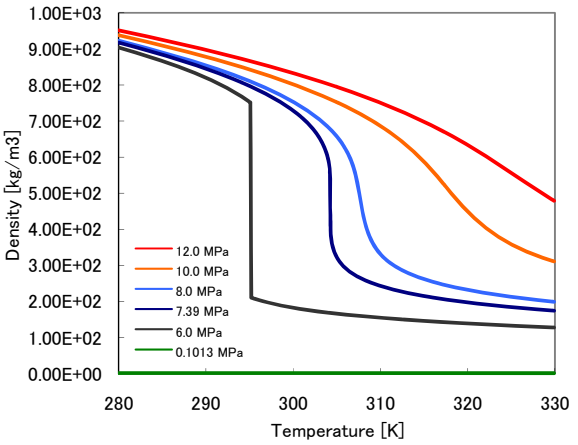


Figure 2 Density values while changing temperature and pressure

The EOS presented in IAPWS IF97 (1999) is known as that for water. Density can be calculated by the EOS as a function of temperature and pressure. Isobaric and isometric specific heats and the related partial derivatives can be also derived from the EOS. As other properties, molecular viscosities and thermal conductivities should be also mathematically modeled. Kyushu University developed a database of thermophysical properties for 48 substances: PROPATH (2008). Most of the mathematical models for EOS, molecular viscosity, thermal conductivity, isobaric and isometric specific heats and so on, are programmed as a polynomial equation which has been standardized by an authorized conference or society.

Figure 3 shows the isobaric specific heat of carbon dioxide while changing temperature and pressure obtained by PROPATH. The value has a maximum

peak at the pseudo-critical temperature as obtained at the pressures of 7.39 and 8.0 MPa. Since the anomalous property is quite deeply related to the flow feature near the critical point, the accurate evaluation is absolutely necessary for simulating supercritical-fluid flows.

Our computational code based on the preconditioning method was fully coupled with PROPATH. Thermophysical properties are programmed as functions for each substance in PROPATH. The set of the functions are contained in a same file as the library file for each substance. The names of the functions are all the same in the different libraries even though the substance is different. This feature enables us to change the substance quite easily. Only if the library file is replaced to the other, our code can simulate thermophysical flows of different substance, such as carbon dioxide, water, nitrogen, hydrogen, methane, and so on. Most distinguished feature is that the present method can simulate supercritical-fluid flows of such substance across the critical point.

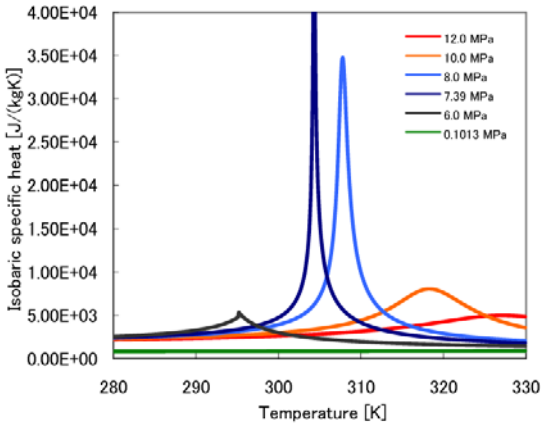
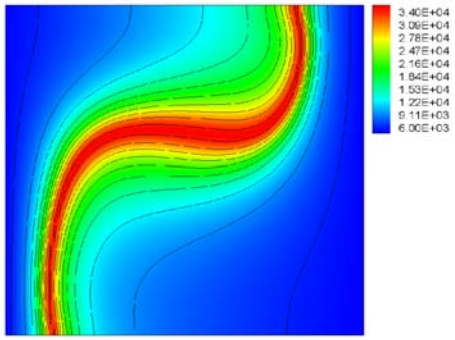


Figure 3 Values of isobaric specific heat while changing temperature and pressure

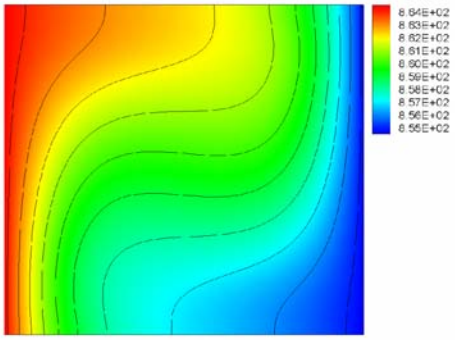
4. Numerical Examples

Our method has been already applied to several practical problems (Yamamoto et al., 2011-1) (Yamamoto et al., 2011-2). Here a simple thermal convection problem indicating the importance of evaluating thermophysical properties is first introduced. Two-dimensional natural convection of carbon dioxide between two parallel plates in a vertical direction is calculated. The numerical results have been already reported by Davis (1983). A case assuming a Rayleigh number of 10^4 in atmospheric pressure and temperature conditions is calculated. The bulk pressure is 0.1[MPa]. The temperatures on the left and right plates are 303 and 313[K], respectively. This case is further extended to natural convection in a supercritical-pressure condition. The pressure is increased to 8.0[MPa]. In this condition, the phase change between supercritical fluid and liquid occurs at an intermediate value of the temperatures between 303 and 313[K].

Figures 4(a) and 4(b) show the calculated distributions of isobaric specific heat at the pressure of 8.0[MPa] and that of 0.1[MPa], respectively. A zonal region where the isobaric specific heat has a maximum peak is captured in Fig. 4(a). Usually the value is almost constant in a gas as obtained in Fig. 4(b). The maximum peak value in Fig.4(a) is approximately seven times higher than the minimum value in Fig. 4(b).



(a) 8.0MPa



(b) 0.1MPa

Figure 4 Calculated isobaric specific heats

Next, two-dimensional natural convection of cold water at approximately 4°C between two parallel plates is calculated. In general, liquid water under atmospheric conditions may be calculated as an incompressible fluid without compressibility. However, although water is in a liquid condition, it has an exact value of trivial compressibility. Anomalous property of cold water at approximately 4°C under atmospheric pressure conditions has been reported by Banaszek et al. (1999). The density of liquid water has a peak value at 4°C because of the structure of the molecular combination between hydrogen and oxygen atoms.

Figure 5 shows the calculated temperature distributions and the corresponding velocity vectors obtained by our method. Figure 6 shows the corresponding density distributions. Although the density difference in the flow field is insignificant, the highest value of density is observed in the region at approximately 4°C. These figures indicate that the higher density region induces a downward flow that is against the buoyancy effect. The experimental and numerical results obtained by Banaszek et al. (1999) indicates that the downward flow makes an additional vortex at the right and bottom corner. The velocity

vectors in Fig.5 show that the additional vortex is obtained in the result. The calculated distributions were quite in good agreement with the experimental data.

Our method has been also applied to a hydro synthesis of supercritical water and a supersonic nozzle flow of supercritical carbon dioxide with expansion chamber.

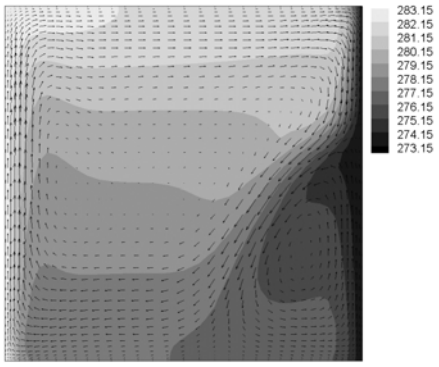


Figure 5 Temperature distributions and velocity vectors

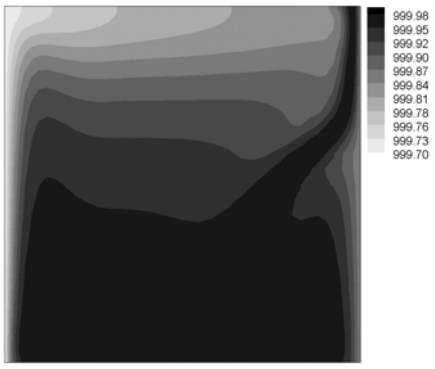


Figure 6 Density distributions

5. Concluding Remarks

Thermophysical flows are one of certain targets for future CFD researches. The main issue is how the thermophysical properties are modelled and programmed in the CFD code. Our study may answer the question. Thermophysical models have been studied in detail by chemical engineers. Employing such models with robust flow solvers is straightforward for simulating thermophysical flows.

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