Numerical Methods for Simulating Supercritical-Fluid Flows over and in Arbitrary Geometry
(Summary)
任意形状物体内外における超臨界流体の数値解法
(要約)

第１章　Introduction

A supercritical fluid (SCF) is any substance at a pressure and temperature beyond its critical point. There are some unique characteristics of supercritical fluids, and a lot of important applications of SCF flows in industrial and engineering fields are proposed because of the superior thermophysical properties. However, despite of the fact above, the physical details of fluid mechanics and thermal dynamics in SCF flows are still not completely understood.

The early studies are mainly basic researches on the heat transfer characteristics in SCF flows such as the SC H_2O or SC CO_2. Recently, there are also some application researches of SCF flows such as the applications in the SCHS process and the HSD process. The difficulties in the study of SCF flows lead to the situation that the experimental researches rarely show the details of fluid mechanics and thermal dynamics in SCF flows, while the numerical studies are also far from expectations because the common numerical methods (commercial codes, for example) are not able to deal with the SCF flow simulations effectively and efficiently. The numerical method designed for the simulation of SCF flows in practical applications is an urgent issue to be solved.

The objective of the present study is to develop a numerical method for simulating SCF flows in practical applications involving arbitrary geometrical configurations and complex physical phenomenon, in which the Supercritical-Fluid Simulator (SFS) has been coupled with the Building-Cube Method (BCM). The SFS is developed by our group which has been demonstrated to be able to deal with the behavior of SCF flows effectively, while the BCM is a blocked-structured Cartesian mesh method which has been demonstrated to be able to deal with the flow simulations in practical applications efficiently. Wall boundary treatment is a critical issue for the numerical methods in SFS and BCM. The commonly used, traditional Cartesian-mesh based wall boundary treatments are tested first with the classical forced convection and natural convection problems in fluid mechanics, which shows the basic validity of the numerical method as well as the limitations of the traditional wall boundary treatments; a least-square meshless-method is further implemented as a wall boundary treatment to deal with the problems of the traditional wall boundary treatments, which further comprises the flexibility and adaptability of the meshless method in the numerical methods in SFS and BCM. The hybrid methods show its great potentials in the design and analysis of SCF flows in practical applications.

第２章　Verification of the numerical methods for simple gases and liquids flows

The basic validity of the numerical methods in SFS and BCM is established for simple gas or liquid flows, and the limitation of the Cartesian-mesh based wall boundary treatment for certain gas or liquid flows is also discussed. The commonly used, traditional wall boundary treatments for the Cartesian mesh are used.

Three Cartesian-mesh based wall boundary treatments are tested for comparisons, and two classical cases in fluid mechanics for gases and liquids are calculated. The forced convection flow past a circular cylinder case shows the different properties of the wall boundary treatments tested, by which the validity of the numerical method with immersed boundary (IB) wall boundary treatment is established; while the natural convection flow over a circular cylinder case further shows the lack of grid resolution problem of the Cartesian-mesh based wall boundary treatment, by which the lack of grid resolution problem for physical gradients resolution was confirmed quantitatively.

For practical applications of either forced convection or natural convection, or both, with significant physical gradients in the wall region, since the grid resolution in the IB method is based on the Cartesian mesh, an extremely fine mesh has to be used, which limits the potential of the IB method to some practical applications of fluid flow problems.

第3章　Verification of the numerical methods for simple supercritical fluid flows

The basic validity of the numerical methods in SFS and BCM is established for simple SCF flows, and the limitation of the Cartesian-mesh based wall boundary treatment for simplified practical SCF flows is further discussed. The IB method is applied as a wall boundary treatment for the Cartesian mesh method.

Three test cases are proposed: the unsteady forced convection flow past two side by side circular cylinders and the natural and forced convection flows over an E-shaped fin cases are calculated first, which shows the similar aerodynamic characteristics and the distinct thermal dynamics in SCF flows, as well as the significant natural convection effect, compared to gases and liquids flows. The mixing flow of supercritical temperature water with room temperature water in a T-shaped channel, which is a simplified SCF flows in practical applications with significant temperature variations is simulated then, which shows the sensitivity of the SCF flows to grid resolution in the Cartesian mesh due to the significant thermophysical property variations. The error due to the non-body-fit feature as well as the lack of grid resolution in physical gradients resolution was further confirmed qualitatively for SCF flows, which indicates the grid resolution limitation might be more severe in SCF flows than for gases and liquids flows.

Though there are also researchers working on the extension of the IB method for further practical applications involving arbitrary geometry and complex physics, a new alternative with body-fit feature of solid wall surface location, as well as the flexibility in dealing with arbitrary geometry and the adaptability in dealing with complex physics should also be considered, for example, the meshless method.

第4章　Investigation of the numerical methods with meshless method based wall boundary treatment

A least-square meshless method is implemented as a wall boundary treatment to deal with the grid resolution limitation in the traditional wall boundary treatments, because of its superior flexibility for arbitrary geometrical configuration and adaptability for complex physical phenomenon.

Three simple test cases in the previous chapters are calculated first to compare the basic property of the meshless method and the IB method as a wall boundary treatment. The forced convection and natural convection flow over a circular cylinder cases show the body-fit feature of the meshless method and its flexibility in the resolution of physical gradients in the wall normal directions for gases and liquid flows; the supercritical mixing flow in a T-shaped channel case shows the advantage of the meshless method over the IB method as a wall boundary treatment for SCF flows. Two complex cases are simulated then to further show the property of the numerical method. The unsteady forced convection flows past two rotating circular cylinders case demonstrates the capability of the numerical method for cases involving complex physics such as the rotating boundary conditions, and the steady and unsteady natural convection flows over a Y-shaped fin case demonstrates the capability of the numerical method for cases involving arbitrary geometry such as the assembly of fin branches.

It has been demonstrated that the numerical method in SFS and BCM with meshless wall boundary treatment comprises the simplicity and efficiency of the Cartesian mesh method, as well as the flexibility and adaptability of the meshless method.

第５章 Application of the numerical methods to practical supercritical fluid flows

The numerical method with meshless wall boundary treatment is extended to the simulation of turbulent flows and three-dimensional flows, and then applied to the simulation of SCF flows in practical applications.

First, a brief verification for turbulence model implementation is proposed, and the capability of the numerical method in the simulation of three-dimensional flows is also validated. Then, the numerical method is applied to the simulation of axisymmetric, turbulent SCF flows in practical applications. The supercritical water jet submerged in a sub critical water environment is calculated, which is a typical process in the hydrothermal spallation drillings (HSD). The numerical results are first compared to the experimental results, in which the effect of jet temperature on the behavior of supercritical water jets is investigated, and then further numerical investigations are proposed in which the effect of system pressure is also investigated. Finally, the numerical method is applied to the simulation of three-dimensional, laminar SCF flows in practical applications. The supercritical hydrothermal synthesis (SCHS) is simulated, which is a typical application of supercritical water for nano-scale particle fabrication. The numerical results are also compared to the experimental results first, and then further numerical investigations on the effects of basic design factors on the behaviors of supercritical water flows in the SCHS reactors are proposed, such as temperature, pressure and mass flow rate, as well as the cross-section shape. In addition, the parallel implementation has also been accomplished for the three-dimensional numerical method, based on the OpenMP strategy.

The potential of the numerical method in the design and analysis of SCF flows in practical applications is clearly demonstrated.

第6章 Conclusions

The basic objective of the present study is to develop a numerical method designed for simulation of SCF flows over and in arbitrary geometry, based on the supercritical-fluid simulator (SFS) and the Cartesian mesh method of BCM. The present method is applicable to real-fluid flow simulations of gases, liquids and supercritical fluids in various conditions, such as the two-dimensional and three-dimensional flows, laminar and turbulent flows etc.

The main challenge is the wall boundary treatment for the Cartesian mesh method in SFS and BCM, and the main contribution is the hybrid numerical methods especially designed for the simulation of SCF flows, showing its great potentials in the design and analysis of SCF flows in practical applications. The hybrid numerical methods comprise the simplicity and efficiency of the Cartesian mesh method, as well as the flexibility and adaptability of the meshless method.

In the future, further application of the numerical method to three-dimensional turbulent SCF flows in practical applications is a key issue. The implementation of the numerical models for multi-physics problems is also a key point to be considered. Finally, the parallel implementation for the meshless method is also a critical issue for further applications.