

**Numerical Analysis of Transport Phenomena  
in Porous Structure  
by the Lattice Boltzmann Method**

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# Chapter 1

## General Introduction

### 1.1 Introductory Remarks

Transport phenomena in porous media are very important subjects in many science and engineering fields. The application of flow and heat/mass transfer in porous media can be found in geophysics, hydraulics, soil mechanics, chemical and petroleum engineering, and so on. In these fields, as for flow in porous media, it is important to estimate the macroscopic properties such as pressure drops or permeability through porous media. As for heat/mass transfer in porous media, on the other hand, the effective thermal conductivities and effective mass diffusivities are needed to many kinds of engineering applications. In chemical engineering applications, for example, knowledge of them is essential to determine the temperature/concentration distributions in a packed bed reactor, in a fuel cell, in a non-isothermal catalyst pellet, in the drying process, and so on. In the past studies volume-averaged technique is usually used to obtain these macroscopic properties. However, when we treat complex porous media with non-uniform porosity, for instance, it is more important to investigate microscopic process occurring at a pore scale and to obtain the properties from the microscopic point of view. In such cases, it is considered that both experimental and theoretical approaches are sometimes

difficult because of complex fluid flows in porous media. Thus, numerical approach will become a powerful and useful tool in these studies.

In the present study the analyses of transport phenomena in porous structures are conducted by a new numerical approach based on the kinetic theory of gases. The approach is the lattice Boltzmann method.

## 1.2 Method of Computations

### 1.2.1 Lattice Boltzmann Method

In recent years, the lattice Boltzmann method (LBM) has developed into an alternative and promising numerical scheme for simulating viscous fluid flows. The method is particularly successful in fluid flow applications involving dynamic interface and complex boundaries. The LBM is different from the conventional numerical approaches, such as finite difference method (FDM) and finite element method (FEM) at a macroscopic level and from the molecular dynamics (MD) simulation at a microscopic level. The LBM is based on microscopic models and mesoscopic kinetic equations. The fundamental idea of the LBM is to construct simplified kinetic models that incorporate the essential physics of the microscopic processes so that the macroscopic properties obey the desired macroscopic equations. The basic premise for using these simplified kinetic-type methods for macroscopic fluid flows is that the macroscopic dynamics of fluid is the result of the collective behavior of many microscopic particles in the system and that the macroscopic dynamics is not sensitive to the underlying details in microscopic physics (Kadanoff 1986).

In the conventional numerical methods, the discretized macroscopic equations are directly solved. Since the macroscopic equations are nonlinear and the solutions of nonlinear equations are highly related to boundaries, it should be very difficult to

solve the equations especially if the physical system has complex geometries such as porous media. Besides, when the continuity equation and the Navier-Stokes equations for incompressible fluid are calculated using the conventional numerical approaches, the pressure satisfies a Poisson equation and solving this equation for the pressure often produces numerical difficulties requiring special treatment, such as iteration or relaxation (e.g. Ferziger & Perić 1996). The MD simulation, on the other hand, can simulate complex fluid phenomena by implementing the correct intermolecular potential. However, the MD simulation requires enormous computational resources and is rather impractical for fluid simulations.

The LBM is a mesoscopic approach, that is, intermediate between the macroscopic and microscopic approaches. Instead of solving the macroscopic nonlinear equations and tracking individual molecules as in the MD simulations, the LBM simulates the fluid flows by solving kinetic equations at the mesoscopic level. In addition, by developing a simplified version of the kinetic equation one can avoid solving complicated kinetic equations such as the full Boltzmann equation. Therefore, the LBM is regarded as an efficient and attractive tool for simulating the fluid flows including complex phenomena.

### 1.2.2 Brief History of LBM

Figure 1.1 shows the brief history of the lattice Boltzmann method. Historically, the LBM evolved from the lattice gas automata (LGA), in which space, time, and particle velocities are all discrete. In the LGA, the physical fluids are first assumed to consist of discrete particles, which reside only on the lattice nodes at discrete time steps. The particles move on the spatial lattice and scatter according to some scattering rules. Frisch, Hasslacher & Pomeau (1986) proposed the first version of LGA, what is called FHP model, on a hexagonal lattice in two-dimensional space

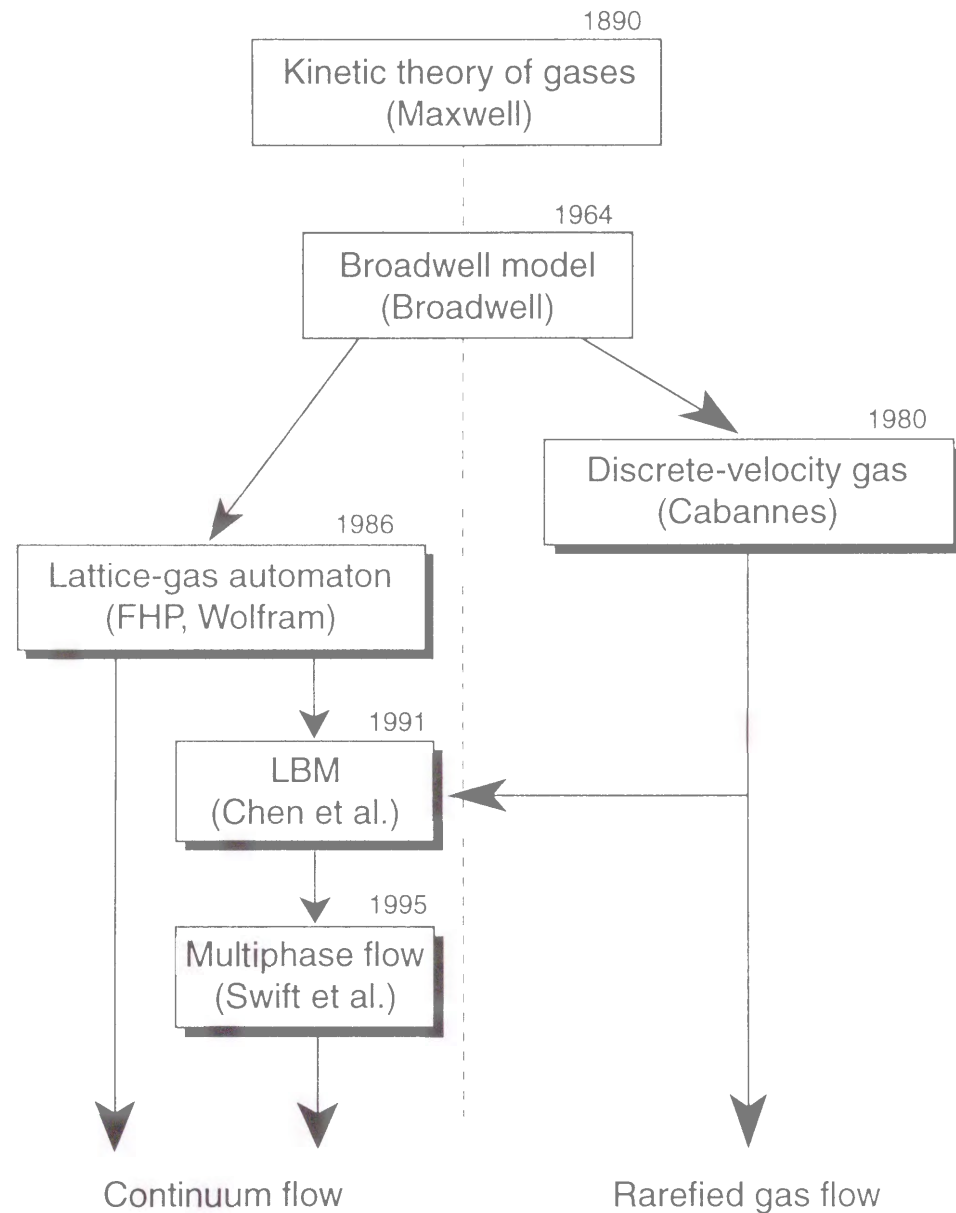


Figure 1.1: History of the lattice Boltzmann method.

and showed that the LGA recovers the isotropic hydrodynamic equations. The central ideas in the papers contemporary with the FHP paper include the cellular automaton model (Wolfram 1986) and the three-dimensional model using the four-dimensional face-centered hypercubic (FCHC) lattice (d'Humières, Lallemand & Frisch 1986).

On the other hand, the LBM can also be regarded as a special finite difference scheme for the kinetic equation of the discrete velocity gas, in which the particle velocity is discretized but space and time are continuous. This kinetic equation is called the discrete Boltzmann equation (DBE) and describes the evolution of particle populations that have discrete velocities. Several researchers have used a variety of discrete particle velocities models. Broadwell (1964) employed the simplified kinetic equation with a single-particle speed model to simulate fluid flows for studying shock structures. In fact, one can regard the Broadwell model as a simple one-dimensional lattice Boltzmann equation (LBE). Inamuro & Sturtevant (1990) have also used multispeed discrete particle velocities models for studying shock-wave structures. Later, Sterling & Chen (1996) derived the LBE by discretizing the Boltzmann equation in spatial and time spaces. The relation of the LBM to kinetic theory was also explored by Abe (1997). All these work are based on the assumption that the underlying discrete velocities are known *a priori* (He, Chen & Doolen 1999).

The first LBM model proposed by McNamara & Zanetti (1988) has the complicated collision operator. An important simplification of the LBM was made by Higuera & Jimenez (1989) who linearized the collision operator by assuming that the distribution is close to the local equilibrium state. Later by two independent groups (Chen *et al.* 1991a; Qian, d'Humières & Lallemand 1992), the collision operator can be further simplified by making the single-relaxation-time approximation.

The relaxation term is known as the Bhatnagar-Gross-Krook (BGK) collision operator (Bhatnagar, Gross & Krook 1954). This so-called lattice BGK model greatly reduces the computational time and memory. What is more important, this model ensures the isotropy and Galilean invariance and possesses a velocity-independent pressure, although the LGA models do not satisfy these requirements and have a velocity-dependent pressure (Chen, H., Chen, S. & Matthaeus 1992). Thus, the lattice BGK model is the most popular form in the LBM. More details are referred to as References, Rothman & Zaleski (1997), Chen & Doolen (1998), He, Chen & Doolen (1999), Tsutahara, Takada & Kataoka (1999), and so on.

### 1.2.3 Applications of LBM

Up to now, the LBM has been successfully applied to many kinds of simulations of viscous flows as follows: fluid flow in complex geometry including porous and random media (Succi, Foti & Higuera 1989; Cancelliere *et al.* 1990; Spaid & Phelan 1997), multiphase and multicomponent fluid flows (Gunstensen *et al.* 1991; Shan & Chen 1994; Swift, Osborn & Yeomans 1995; Swift *et al.* 1996; Inamuro, Konishi & Ogino 1999; Inamuro, Miyahara & Ogino 2000), turbulent flows (Martínez *et al.* 1994; Benzi, Struglia & Tripiccone 1996), suspension, colloidal, and granular flow (Aidun & Lu 1995; Ladd 1994, 1997), heat transfer (McNamara, Garcia & Alder 1997; Chen, Ohashi & Akiyama 1997; Shan 1997; He, Chen & Doolen 1998), reactive and diffusion system (Cali *et al.* 1992; Holme & Rothman 1992; Dawson, Chen & Doolen 1993; Chen *et al.* 1995), and many others.

### 1.2.4 Challenging Issues on LBM

As mentioned above, the LBM has been used for a variety of applications in recent years. Although the great success of the LBM has been achieved, there remain

challenging issues to be well studied. In the following, a couple of important topics, the relation between the LBE and the continuity equation and the Navier-Stokes equations for incompressible fluid, the accuracy of the LBM to the fluid-dynamic type equations, and boundary conditions in the LBM, are given.

### Derivation of Fluid-Dynamic Type Equations and Accuracy of LBM

To derive the fluid-dynamic type equation from the LBE, one usually employs the Chapman-Enskog expansion procedure, which is essentially a formal multiscale expansion (Frisch *et al.* 1987). The Chapman-Enskog expansion procedure is an asymptotic expansion method for solving the Boltzmann equation in the kinetic theory of gases. In general, however, the derivation of the continuity equation and the Navier-Stokes equations for incompressible fluid from the LBE by using this procedure contains some kinds of assumptions and is not so clear and successful.

Likewise, in the investigation of the accuracy of the LBM to the fluid-dynamic type equations, the Chapman-Enskog expansion procedure is also usually used for the LBE and it has been found that the LBE approaches the Navier-Stokes equations with error terms proportional to the Knudsen number squared and Mach number cubed (Hou *et al.* 1995; Zou *et al.* 1995; Sterling & Chen 1996). These errors are referred to generally as compressibility error. Since the Knudsen number is related to lattice resolution by the relaxation time (Hou *et al.* 1995), it is said that the accuracy of the LBM depends on the Knudsen number, Mach number, and lattice resolution. However, Maier, Bernard & Grunau (1996) have pointed out that neither the Mach number nor Knudsen number is separately a good index for error estimates with a duct flow problem and that the product of Mach and Knudsen numbers is a fairly good index for the error estimates. Moreover, Reider & Sterling (1995) have

pointed out that for a fix Mach number the calculated result by LBM converges to a certain solution that is different from the solution of the incompressible Navier–Stokes equations, as lattice spacing is reduced. It is found from the above facts that the error estimates of LBM based on the Chapman–Enskog expansion procedure have not been so clear and successful.

Therefore, another way to derive the continuity equation and the Navier–Stokes equations for incompressible fluid from the LBE and to estimate the accuracy of LBM to the fluid-dynamic type equations is needed.

### Boundary Conditions in LBM

Wall boundary conditions in the LBM were originally borrowed from the LGA. In the LBM, the bounce-back boundary condition (d’Humières & Lallemand 1987) has been usually used to model stationary walls. Under the bounce-back rule, all the particles colliding with walls are reflected back in the direction from which they came. However, it has been found that the bounce-back boundary condition has errors in velocity at the wall (Noble *et al.* 1995; Ziegler 1993; Ginzbourg & Adler 1994). In general, the velocity along the wall obtained by using this boundary condition is not equal to that of the wall velocity. The difference between the fictitious velocity and the wall velocity is called the slip velocity. Skordos (1993) proposed a method for calculating particle distributions at a boundary node from fluid variables with the gradients of the fluid velocity. In his method the density is assumed to be known at the boundary. Noble *et al.* (1995) developed a method for calculating the density at the boundary and the unknown components of the particle distributions. While their method gives accurate results with the seven-velocity model, it is not clear whether the method can be applied to other velocity

models. Maier *et al.* (1996) modified the bounce-back condition to nullify net momentum tangent to the wall and to preserve momentum normal to the wall. Zou & He (1997) extended the bounce-back condition for the nonequilibrium portion of the distribution. It appears, however, that the extension of these simple assumptions to arbitrary boundary conditions is difficult. Therefore, a new boundary condition which can accurately model any no-slip wall is needed.

## 1.3 Summary of Previous Studies

In the past studies on transport phenomena in porous media, volume-averaged approaches are usually used to obtain macroscopic properties, such as pressure drops or permeabilities, effective thermal conductivities, and effective mass diffusivities in porous media. In order to estimate pressure drops in porous media, for example, the Blake–Kozeny equation (Bird, Stewart & Lightfoot 1960) and the Ergun equation (Ergun 1952), which are both empirical equations based on experimental data, are often used for low and high Reynolds numbers, respectively. In recent experimental works, Fand *et al.* (1987) studied flow through porous media composed of randomly packed spheres and proposed the useful correlation equations between pressure gradients and flow velocities. Liu, Afacan & Masliyah (1994) studied laminar flows in porous media and presented a new averaging approach to the pressure gradient term. However, in these studies the relation between flow fields at a pore scale and pressure drops has not been so clear. As for the studies on flow characteristics, Dybbs & Edwards (1984) carried out experiments of liquid flow in porous media consisting of plexiglas spheres in a close hexagonal packing and cylindrical rods in a complex geometrical structure. They classified flow characteristics into four flow regimes: Darcy or creeping flow regime, inertial flow regime, unsteady laminar flow

regime, and highly unsteady and chaotic flow regime. However, more quantitative investigations are needed to make clear flow characteristics in porous media.

In numerical simulations, on the other hand, previous studies, including finite-difference schemes (Schwarz *et al.* 1993) and networking models (Koplik & Lasseeter 1984), were either limited to simple physics, small geometry size, or both. Buonomano & Carotenuto (1997) proposed a method to calculate the effective thermal conductivity of a two-phase isotropic porous medium by means of a volume-averaged technique. As for the LGA and LBM, Rothman (1988) used the LGA for simulations of flow through porous media and verified Darcy's law (a linear relation between the pressure gradient and the volume flow rate per unit area) in simple and complicated geometries. Chen *et al.* (1991b) also used the LGA to study microscopic behaviors occurring at a pore scale and to obtain volume-averaged parameters from the microscopic point of view. Succi, Foti & Higuera (1989) utilized the LBM to measure the permeability in a three-dimensional random media. Darcy's law was confirmed. Cancelliere *et al.* (1990) studied the permeability as a function of solid fraction in a system of randomly positioned spheres of equal radii using the LBM. However, the above-mentioned simulations by the LGA and LBM were applied for relatively low Reynolds numbers and restricted to laminar flow regions. In recent years, Inamuro, Yamamura & Ogino (1995) have investigated the problems of flow and heat transfer in a two-dimensional porous structure for low and high Reynolds numbers by using the LBM. They conclude that the method is useful for studying microscopic properties of flow and heat transfer problems, although more quantitative investigations are needed due to the two-dimensional simulations. Thus, it is desired to study three-dimensional problems of flow and heat/mass transfer in porous media at high Reynolds numbers as well as low Reynolds numbers.

## 1.4 Objectives and Outline of this Thesis

The final objectives of this study are to develop the LBM for simulations of fluid flow problems and flow and mass transfer problems in a three-dimensional porous structure and to investigate the transport phenomena in the structure from the microscopic point of view.

Chapter 2 deals with the fundamentals of the LBM. First, the relation between the lattice Boltzmann equation and the continuity equation and the Navier-Stokes equations for incompressible fluid is clarified. In addition, the accuracy of the LBM to the fluid-dynamic type equations is investigated. Next, boundary conditions in the LBM are discussed. Finally, the LBM for a binary fluid mixture with a simple kinetic model is proposed.

Chapter 3 deals with numerical analysis of flows in a three-dimensional porous structure. Flow fields at a pore scale and pressure drops through the structure are calculated for various Reynolds numbers. The calculated pressure drops are compared with well-known empirical equations based on experimental data. Also, the characteristics of the unsteady flows in the structure at relatively high Reynolds numbers are investigated.

Chapter 4 deals with numerical analysis of flow and mass transfer for a binary fluid mixture in the porous structure. Flow characteristics and concentration profiles of diffusing component at a pore scale are simulated for various Reynolds numbers. In addition, Sherwood numbers are calculated and compared with available experimental data for packed beds.

Chapter 5 finally gives the conclusion of this thesis. Remarks and recommendations for further studies are also given.

## Chapter 2

# Lattice Boltzmann Method

### 2.1 Introduction

In this Chapter, basic theories for the lattice Boltzmann method (LBM) are introduced. As mentioned in Section 1.2.4, there have been a couple of challenging issues to be well discussed in the LBM. Hence, first of all, the S-expansion procedure of the asymptotic theory proposed by Sone (Sone 1971, 1991; Sone & Aoki 1994) is applied to the LBM with the fifteen-velocity model and the continuity equation and the Navier–Stokes equations for incompressible fluid are derived. In addition, the accuracy of the LBM to the fluid-dynamic type equations is investigated. Next, boundary conditions in the LBM are studied. A new approach for applying a no-slip boundary condition at wall is proposed. A periodic boundary condition with pressure difference at inlet and outlet is also presented. These boundary conditions are applicable for simulations of flows through the porous structure in the following Chapters 3 and 4. Then, the LBM for a binary fluid mixture with a simple kinetic model is proposed and governing equations for macroscopic variables are obtained by means of the S-expansion procedure. Finally, two fundamental problems are calculated to demonstrate the validity of the above-mentioned methods.

### 2.2 Basic Theories for LBM

#### 2.2.1 Basic Equation

In the following, let  $L$  be a characteristic length,  $U$  a characteristic flow speed, and  $c$  a characteristic particle speed which is of the order of sound speed of the modeled gas. Since incompressible fluid flows are considered, a characteristic time scale  $t_0 = L/U$  is used.

#### Basic Equation of Discrete-Velocity Gas

A modeled gas composed of identical particles whose velocities are restricted to a finite set of  $N$  vectors,  $\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_N$ , is considered. If the Bhatnagar, Gross, and Krook (BGK) model (Bhatnagar, Gross & Krook 1954) is used for collision terms, the behavior of the particles is described by the following discrete Boltzmann equations (DBE) for the particle velocity distribution functions  $f_i$ :

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -A_c \rho (f_i - f_i^{\text{eq}}) \quad \text{for } i = 1, 2, \dots, N, \quad (2.2.1)$$

where  $f_i^{\text{eq}}$  is an equilibrium distribution function,  $A_c$  is a constant, and  $\rho$  is the density of the particles defined below. It is noted that  $A_c \rho$  is the collision frequency of the particles. As in the kinetic theory of gases, we define density  $\rho$ , flow velocity  $\mathbf{u}$ , and internal energy  $e$  in terms of the particle distribution function as follows:

$$\rho = \sum_{i=1}^N f_i, \quad (2.2.2)$$

$$\mathbf{u} = \frac{1}{\rho} \sum_{i=1}^N f_i \mathbf{c}_i, \quad (2.2.3)$$

$$c = \frac{1}{2\rho} \sum_{i=1}^N f_i (\mathbf{c}_i - \mathbf{u}) \cdot (\mathbf{c}_i - \mathbf{u}), \quad (2.2.4)$$

and also we define pressure  $p$  in  $D$ -dimensional space by

$$p = \frac{2}{D} \rho c. \quad (2.2.5)$$

Equations (2.2.1)–(2.2.5) can be written in non-dimensional forms by using characteristic quantities  $L$ ,  $c$ , and  $t_0$  and a reference density  $\rho_0$ . The resulting non-dimensional equations are

$$\text{Sh} \frac{\partial f_i}{\partial t} + \hat{\mathbf{c}}_i \cdot \nabla f_i = -\frac{1}{\epsilon} \hat{\rho} (\hat{f}_i - \hat{f}_i^{\text{eq}}) \quad \text{for } i = 1, 2, \dots, N, \quad (2.2.6)$$

$$\hat{\rho} = \sum_{i=1}^N \hat{f}_i. \quad (2.2.7)$$

$$\hat{\mathbf{u}} = \frac{1}{\hat{\rho}} \sum_{i=1}^N \hat{f}_i \hat{\mathbf{c}}_i. \quad (2.2.8)$$

$$\hat{c} = \frac{1}{2\hat{\rho}} \sum_{i=1}^N \hat{f}_i (\hat{\mathbf{c}}_i - \hat{\mathbf{u}}) \cdot (\hat{\mathbf{c}}_i - \hat{\mathbf{u}}). \quad (2.2.9)$$

$$\hat{p} = \frac{2}{D} \hat{\rho} \hat{c}. \quad (2.2.10)$$

where  $\hat{\mathbf{c}}_i = \mathbf{c}_i/c$ ,  $\hat{\mathbf{x}} = \mathbf{x}/L$ ,  $\hat{t} = t/t_0$ ,  $\hat{f}_i = f_i/\rho_0$ ,  $\hat{\rho} = \rho/\rho_0$ ,  $\hat{\mathbf{u}} = \mathbf{u}/c$ ,  $\hat{c} = c/c^2$ ,  $\hat{p} = p/(\rho_0 c^2)$ ,  $\text{Sh} = L/(t_0 c)$ , and  $\epsilon = c/(A_c \rho_0 L)$ . It is noted that  $\text{Sh}$  is the Strouhal number (Sone & Aoki 1994) and the dimensionless number  $\epsilon$  is of the same order as the Knudsen number. In the following three-dimensional fluid flows are considered. For three-dimensional problems, the fifteen-velocity model (Qian, d'Humières &

Lallemand 1992), shown in Figure 2.1, is usually used. The fifteen-velocity model has the following velocity vectors:

$$\begin{aligned} & [\hat{\mathbf{c}}_1, \hat{\mathbf{c}}_2, \hat{\mathbf{c}}_3, \hat{\mathbf{c}}_4, \hat{\mathbf{c}}_5, \hat{\mathbf{c}}_6, \hat{\mathbf{c}}_7, \hat{\mathbf{c}}_8, \hat{\mathbf{c}}_9, \hat{\mathbf{c}}_{10}, \hat{\mathbf{c}}_{11}, \hat{\mathbf{c}}_{12}, \hat{\mathbf{c}}_{13}, \hat{\mathbf{c}}_{14}, \hat{\mathbf{c}}_{15}] \\ &= \begin{bmatrix} 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \end{bmatrix}. \end{aligned} \quad (2.2.11)$$

On the basis of the Maxwell Boltzmann equilibrium distribution function up to  $O(u^2)$  by using a small Mach number expansion (He & Luo 1997; Abe 1997), an equilibrium distribution function of this model is given by

$$\hat{f}_i^{\text{eq}} = E_i \hat{\rho} \left[ 1 + 3\hat{\mathbf{c}}_i \cdot \hat{\mathbf{u}} + \frac{9}{2} (\hat{\mathbf{c}}_i \cdot \hat{\mathbf{u}})^2 - \frac{3}{2} \hat{\mathbf{u}} \cdot \hat{\mathbf{u}} \right] \quad \text{for } i = 1, 2, 3, \dots, 15. \quad (2.2.12)$$

where

$$E_1 = 2/9,$$

$$E_2 = E_3 = E_4 = E_5 = E_6 = E_7 = 1/9,$$

and

$$E_8 = E_9 = E_{10} = E_{11} = E_{12} = E_{13} = E_{14} = E_{15} = 1/72.$$

It should be noted that a velocity model in the LBM must have discrete particle velocities enough to satisfy the requirements of isotropy, Galilean-invariance, and velocity-independent pressure. In practical calculations, on the other hand, it is clearly desirable that a model with only a small number of particle velocities is used for the reduction of computational time and memory. As shown later in Section 2.2.2, the fifteen-velocity model satisfies these requirements in spite of no more than 15 particle velocities. Therefore, the fifteen-velocity model is regarded as a fairly suitable model for three-dimensional problems.

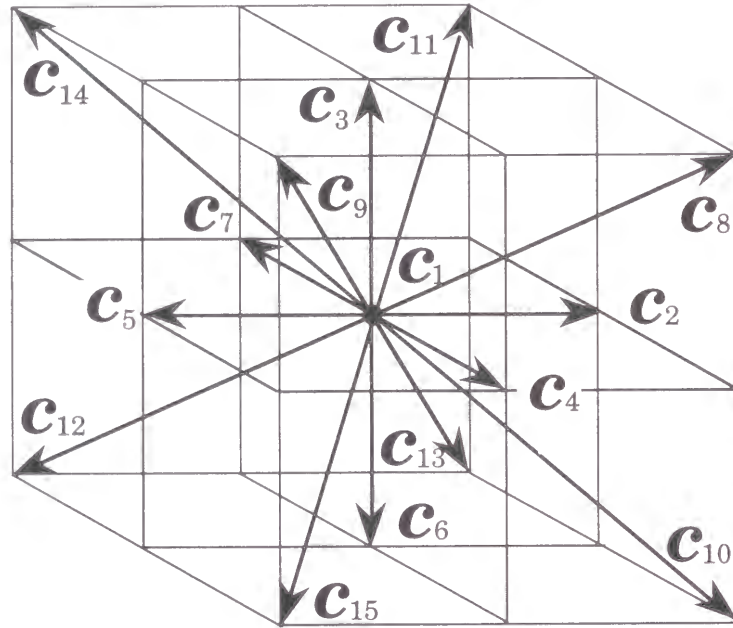


Figure 2.1: Fifteen-velocity model.

## Lattice Boltzmann Equation

In the LBM with the fifteen-velocity model the physical space is divided into a cubic lattice spacing  $\Delta x$ , and a time step is chosen as  $\Delta t = \Delta x/c$ . Thus,  $\Delta \hat{x}_1 = \Delta \hat{x}_2 = \Delta \hat{x}_3 = \Delta \hat{x} (= \Delta x/L)$  and  $\Delta \hat{t}/\text{Sh} = \Delta \hat{x}$ . It should be noted that  $\Delta \hat{x}$  is assumed to be of the same order as  $\epsilon$ . By using a first order upwind discretization of the left-hand side of Equation (2.2.6), the lattice Boltzmann equation (LBE) is obtained as follows:

$$\hat{f}_i(\hat{\mathbf{x}} + \hat{\mathbf{c}}_i \Delta \hat{x}, \hat{t} + \Delta \hat{t}) - \hat{f}_i(\hat{\mathbf{x}}, \hat{t}) = -\frac{1}{\tau} \hat{\rho}(\hat{\mathbf{x}}, \hat{t}) [\hat{f}_i(\hat{\mathbf{x}}, \hat{t}) - \hat{f}_i^{\text{eq}}(\hat{\mathbf{x}}, \hat{t})], \quad (2.2.13)$$

where

$$\tau = \frac{\epsilon}{\Delta \hat{x}}. \quad (2.2.14)$$

It is noted that  $\tau$  is a dimensionless single relaxation time and is of  $O(1)$ .

### 2.2.2 Asymptotic Analysis

The S-expansion procedure of the asymptotic theory proposed by Sone is applied to the LBM with the fifteen-velocity model and fluid-dynamic type equations are obtained. In the analysis, macroscopic variables as well as distribution functions are expanded in the series of small Knudsen number taking into account the relation among Knudsen, Reynolds, and Mach numbers, although in the Chapman–Enskog theory macroscopic variables are not expanded. The expansion of macroscopic variables is useful for error estimates of the LBM, since the ordering of each term in governing equations for macroscopic variables is easily treated.

## Fluid-Dynamic Type Equations

In the kinetic theory of gases, Mach number  $\text{Ma}$  and Knudsen number  $\text{Kn}$  are usually defined by  $\text{Ma} = U/c_0$  and  $\text{Kn} = \bar{c}/(A_c \rho_0 L)$ , where  $c_0$  is the speed of sound and  $c$  is the mean particle speed of the equilibrium state at rest. However, since we are interested only in ordering, the Mach number and Knudsen number defined by  $\text{Ma} = U/c$  and  $\text{Kn} = c/(A_c \rho_0 L) = \epsilon$  are used in the following.

Here, we are interested in the case of a small Knudsen number with finite Reynolds number. Since the Mach number  $\text{Ma}$ , Reynolds number  $\text{Re} = \rho_0 U L / \mu$  ( $\mu$  is the viscosity of fluid), and Knudsen number  $\text{Kn}$  are related as  $\text{Ma} \sim \text{Kn} \text{Re}$  (a definite relation is given later in Equation (2.2.49)), it follows that  $\text{Ma}$  is of the same order as  $\text{Kn}$  in the case of a finite Reynolds number. In addition, since  $\text{Sh} = U/c = \text{Ma}$ , the Strouhal number  $\text{Sh}$  is also of the order of  $\text{Kn}$ . Considering this ordering, we carry out the asymptotic analysis for small Knudsen numbers according to References, Sone (1971, 1991) and Sone & Aoki (1994).

First, performing a Taylor expansion of the left-hand side of Equation (2.2.13) around  $\hat{\mathbf{x}}$  and  $\hat{t}$ , we obtain

$$\begin{aligned} f_i(\mathbf{x} + \hat{\mathbf{c}}_i \Delta \hat{x}, \hat{t} + \Delta \hat{t}) - \hat{f}_i(\hat{\mathbf{x}}, \hat{t}) \\ = d\hat{f}_i(\hat{\mathbf{x}}, \hat{t}) + \frac{1}{2!} d^2 \hat{f}_i(\hat{\mathbf{x}}, \hat{t}) + \frac{1}{3!} d^3 \hat{f}_i(\hat{\mathbf{x}}, \hat{t}) + \dots, \end{aligned} \quad (2.2.15)$$

where

$$d^n = \left( (\Delta \hat{x}) \hat{\mathbf{c}}_i \cdot \hat{\nabla} + (\Delta \hat{t}) \frac{\partial}{\partial \hat{t}} \right)^n \quad \text{for } n = 1, 2, 3, \dots, \quad (2.2.16)$$

Here, we use the aforementioned relation,  $\Delta \hat{t} = \text{Sh} \Delta \hat{x}$ , and retain terms in Equation (2.2.15) up to  $O[(\Delta \hat{x})^3]$ . Then, substituting the resulting equation into Equation

(2.2.13), we have

$$\begin{aligned} (\Delta \hat{x}) \left( \text{Sh} \frac{\partial}{\partial \hat{t}} + \hat{\mathbf{c}}_i \cdot \hat{\nabla} \right) \hat{f}_i + (\Delta \hat{x})^2 \left( \text{Sh} \frac{\partial}{\partial \hat{t}} + \frac{1}{2} \hat{\mathbf{c}}_i \cdot \hat{\nabla} \right) (\hat{\mathbf{c}}_i \cdot \hat{\nabla}) \hat{f}_i \\ + \frac{1}{6} (\Delta \hat{x})^3 (\hat{\mathbf{c}}_i \cdot \hat{\nabla})^3 \hat{f}_i + O[(\Delta \hat{x})^4] = -\frac{1}{\tau} \rho (f_i - \hat{f}_i^{\text{eq}}). \end{aligned} \quad (2.2.17)$$

Next, we put  $\hat{f}_i$  in the form of series expansion of a small parameter  $k$ ,

$$\hat{f}_i = E_i (1 + k \hat{f}_i^{(1)} + k^2 \hat{f}_i^{(2)} + k^3 \hat{f}_i^{(3)} + k^4 \hat{f}_i^{(4)} + \dots) \quad \text{for } i = 1, 2, 3, \dots, 15. \quad (2.2.18)$$

where  $k$  is of the same order as  $\Delta \hat{x}$  and is related to  $\tau$ . The  $k$  is regarded as a modified Knudsen number. It should be noted that the first term of the expansion (the constant term) represents the equilibrium state at rest with the density  $\rho_0$ , so that the deviation of  $\hat{f}_i$  from the equilibrium state at rest is assumed to be of the order of  $\text{Kn}$  (S-expansion). Corresponding to Equation (2.2.18), the macroscopic variables are also expanded as follows:

$$\hat{\rho} = 1 + k \hat{\rho}^{(1)} + k^2 \hat{\rho}^{(2)} + k^3 \hat{\rho}^{(3)} + \dots, \quad (2.2.19a)$$

$$\hat{\mathbf{u}} = k \hat{\mathbf{u}}^{(1)} + k^2 \hat{\mathbf{u}}^{(2)} + k^3 \hat{\mathbf{u}}^{(3)} + \dots, \quad (2.2.19b)$$

$$\hat{c} = \frac{1}{2} + k \hat{c}^{(1)} + k^2 \hat{c}^{(2)} + k^3 \hat{c}^{(3)} + \dots, \quad (2.2.19c)$$

$$\hat{p} = \frac{1}{3} + k \hat{p}^{(1)} + k^2 \hat{p}^{(2)} + k^3 \hat{p}^{(3)} + \dots, \quad (2.2.19d)$$

where

$$\hat{\rho}^{(1)} = \sum_{i=1}^{15} E_i \hat{f}_i^{(1)}, \quad (2.2.20a)$$

$$\hat{\mathbf{u}}^{(1)} = \sum_{i=1}^{15} E_i \hat{f}_i^{(1)} \hat{\mathbf{c}}_i, \quad (2.2.20b)$$

$$c^{(1)} = \frac{1}{2} \sum_{i=1}^{15} E_i \hat{f}_i^{(1)} \hat{\mathbf{c}}_i \cdot \hat{\mathbf{c}}_i - \frac{1}{2} \hat{\rho}^{(1)}. \quad (2.2.20c)$$

$$p^{(1)} = \frac{1}{3} \hat{\rho}^{(1)} + \frac{2}{3} c^{(1)}. \quad (2.2.20d)$$

$$\rho^{(2)} = \sum_{i=1}^{15} E_i \hat{f}_i^{(2)}. \quad (2.2.21a)$$

$$\mathbf{u}^{(2)} = \sum_{i=1}^{15} E_i \hat{f}_i^{(2)} \hat{\mathbf{c}}_i - \hat{\rho}^{(1)} \mathbf{u}^{(1)}. \quad (2.2.21b)$$

$$c^{(2)} = \frac{1}{2} \sum_{i=1}^{15} E_i \hat{f}_i^{(2)} \hat{\mathbf{c}}_i \cdot \hat{\mathbf{c}}_i - \frac{1}{2} \hat{\rho}^{(2)} - \hat{\rho}^{(1)} c^{(1)} - \frac{1}{2} \mathbf{u}^{(1)} \cdot \mathbf{u}^{(1)}, \quad (2.2.21c)$$

$$p^{(2)} = \frac{1}{3} \hat{\rho}^{(2)} + \frac{2}{3} \hat{\rho}^{(1)} c^{(1)} + \frac{2}{3} c^{(2)}. \quad (2.2.21d)$$

$$\rho^{(3)} = \sum_{i=1}^{15} E_i \hat{f}_i^{(3)}, \quad (2.2.22a)$$

$$\mathbf{u}^{(3)} = \sum_{i=1}^{15} E_i \hat{f}_i^{(3)} \hat{\mathbf{c}}_i - \hat{\rho}^{(1)} \mathbf{u}^{(2)} - \hat{\rho}^{(2)} \mathbf{u}^{(1)}, \quad (2.2.22b)$$

$$c^{(3)} = \frac{1}{2} \sum_{i=1}^{15} E_i \hat{f}_i^{(3)} \hat{\mathbf{c}}_i \cdot \hat{\mathbf{c}}_i - \frac{1}{2} \hat{\rho}^{(3)} - \hat{\rho}^{(1)} c^{(2)} - \hat{\rho}^{(2)} c^{(1)} - \mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)} - \frac{1}{2} \hat{\rho}^{(1)} \mathbf{u}^{(1)} \cdot \mathbf{u}^{(1)}, \quad (2.2.22c)$$

$$p^{(3)} = \frac{1}{3} \hat{\rho}^{(3)} + \frac{2}{3} \hat{\rho}^{(1)} c^{(2)} + \frac{2}{3} \hat{\rho}^{(2)} c^{(1)} + \frac{2}{3} c^{(3)}. \quad (2.2.22d)$$

It should be noted that the leading term of the expansion for the fluid velocity is of the order of  $k$  because Ma is of the order of Kn. Also, the equilibrium distribution function is expanded as follows:

$$\hat{f}_i^{\text{eq}} = E_i (1 + k \hat{f}_i^{\text{eq}(1)} + k^2 \hat{f}_i^{\text{eq}(2)} + k^3 \hat{f}_i^{\text{eq}(3)} + k^4 \hat{f}_i^{\text{eq}(4)} + \dots) \quad \text{for } i = 1, 2, 3, \dots, 15, \quad (2.2.23)$$

where

$$\hat{f}_i^{\text{eq}(1)} = \hat{\rho}^{(1)} + 3 \mathbf{c}_i \cdot \mathbf{u}^{(1)}, \quad (2.2.24a)$$

$$\begin{aligned} \hat{f}_i^{\text{eq}(2)} &= \hat{\rho}^{(2)} + 3 \hat{\rho}^{(1)} \mathbf{c}_i \cdot \mathbf{u}^{(1)} + 3 \hat{\mathbf{c}}_i \cdot \mathbf{u}^{(2)} \\ &\quad + \frac{9}{2} (\mathbf{c}_i \cdot \mathbf{u}^{(1)})^2 - \frac{3}{2} \mathbf{u}^{(1)} \cdot \mathbf{u}^{(1)}. \end{aligned} \quad (2.2.24b)$$

$$\begin{aligned} \hat{f}_i^{\text{eq}(3)} &= \hat{\rho}^{(3)} + 3 \hat{\rho}^{(2)} \mathbf{c}_i \cdot \mathbf{u}^{(1)} + 3 \hat{\rho}^{(1)} \hat{\mathbf{c}}_i \cdot \mathbf{u}^{(2)} + 3 \mathbf{c}_i \cdot \mathbf{u}^{(3)} \\ &\quad + \frac{9}{2} \hat{\rho}^{(1)} (\hat{\mathbf{c}}_i \cdot \mathbf{u}^{(1)})^2 + 9 (\hat{\mathbf{c}}_i \cdot \mathbf{u}^{(1)}) (\mathbf{c}_i \cdot \mathbf{u}^{(2)}) \\ &\quad - \frac{3}{2} \hat{\rho}^{(1)} \mathbf{u}^{(1)} \cdot \mathbf{u}^{(1)} - 3 \mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)}. \end{aligned} \quad (2.2.24c)$$

$$\begin{aligned} \hat{f}_i^{\text{eq}(4)} &= \hat{\rho}^{(4)} + 3 \hat{\rho}^{(3)} \mathbf{c}_i \cdot \mathbf{u}^{(1)} + 3 \hat{\rho}^{(2)} \hat{\mathbf{c}}_i \cdot \mathbf{u}^{(2)} + 3 \hat{\rho}^{(1)} \mathbf{c}_i \cdot \mathbf{u}^{(3)} + 3 \mathbf{c}_i \cdot \mathbf{u}^{(4)} \\ &\quad + \frac{9}{2} \hat{\rho}^{(2)} (\hat{\mathbf{c}}_i \cdot \mathbf{u}^{(1)})^2 + 9 \hat{\rho}^{(1)} (\mathbf{c}_i \cdot \mathbf{u}^{(1)}) (\hat{\mathbf{c}}_i \cdot \mathbf{u}^{(2)}) \\ &\quad + \frac{9}{2} (\hat{\mathbf{c}}_i \cdot \mathbf{u}^{(2)})^2 + 9 (\hat{\mathbf{c}}_i \cdot \mathbf{u}^{(1)}) (\mathbf{c}_i \cdot \mathbf{u}^{(3)}) \\ &\quad - \frac{3}{2} \hat{\rho}^{(2)} \mathbf{u}^{(1)} \cdot \mathbf{u}^{(1)} - 3 \hat{\rho}^{(1)} \mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)} \\ &\quad - \frac{3}{2} \mathbf{u}^{(2)} \cdot \mathbf{u}^{(2)} - 3 \mathbf{u}^{(1)} \cdot \mathbf{u}^{(3)}. \end{aligned} \quad (2.2.24d)$$

We consider a moderately varying solution [ $\partial f_i / \partial t = O(f_i)$  and  $\partial f_i / \partial x_\alpha = O(f_i)$  with  $\alpha = 1, 2, 3$  ( $\alpha$  : Cartesian coordinate)] of Equation (2.2.17). Substituting Equations (2.2.18) and (2.2.23) into Equation (2.2.17), we obtain the following simultaneous equations governing the component functions  $\hat{f}_i^{(m)}$  ( $m = 1, 2, 3, \dots$ ) of the velocity distribution functions  $\hat{f}_i$ :

$$\hat{f}_i^{(1)} = \hat{f}_i^{\text{eq}(1)}, \quad (2.2.25)$$

$$\hat{f}_i^{(2)} = \hat{f}_i^{\text{eq}(2)} - \frac{\tau \Delta x}{k} \hat{\mathbf{c}}_i \cdot \nabla \hat{f}_i^{(1)} - \hat{\rho}^{(1)} (\hat{f}_i^{(1)} - \hat{f}_i^{\text{eq}(1)}), \quad (2.2.26)$$

$$\hat{f}_i^{(3)} = \hat{f}_i^{\text{eq}(3)} - \frac{\tau \Delta x}{k} \hat{\mathbf{c}}_i \cdot \nabla \hat{f}_i^{(2)}$$

$$\begin{aligned}
& -\frac{\tau\Delta x}{k}\left[\frac{\text{Sh}}{k}\frac{\partial}{\partial t}+\frac{1}{2}\left(\frac{\Delta x}{k}\right)(\hat{\mathbf{c}}_i\cdot\hat{\nabla})^2\right]\hat{f}_i^{(1)} \\
& -\rho^{(1)}(\hat{f}_i^{(2)}-\hat{f}_i^{\text{eq}(2)})-\hat{\rho}^{(2)}(\hat{f}_i^{(1)}-\hat{f}_i^{\text{eq}(1)}), \tag{2.2.27}
\end{aligned}$$

$$\begin{aligned}
\hat{f}_i^{(1)} &= \hat{f}_i^{\text{eq}(1)}-\frac{\tau\Delta x}{k}\hat{\mathbf{c}}_i\cdot\hat{\nabla}\hat{f}_i^{(3)} \\
& -\frac{\tau\Delta x}{k}\left[\frac{\text{Sh}}{k}\frac{\partial}{\partial t}+\frac{1}{2}\left(\frac{\Delta x}{k}\right)(\hat{\mathbf{c}}_i\cdot\hat{\nabla})^2\right]\hat{f}_i^{(2)} \\
& -\left(\frac{\tau\Delta x}{k}\right)^2(\hat{\mathbf{c}}_i\cdot\hat{\nabla})\left[\frac{\text{Sh}}{k}\frac{\partial}{\partial t}+\frac{1}{6}\left(\frac{\Delta x}{k}\right)(\hat{\mathbf{c}}_i\cdot\hat{\nabla})^2\right]\hat{f}_i^{(1)} \\
& -\hat{\rho}^{(1)}(\hat{f}_i^{(3)}-\hat{f}_i^{\text{eq}(3)})-\hat{\rho}^{(2)}(\hat{f}_i^{(2)}-\hat{f}_i^{\text{eq}(2)})-\hat{\rho}^{(3)}(\hat{f}_i^{(1)}-\hat{f}_i^{\text{eq}(1)}). \tag{2.2.28}
\end{aligned}$$

⋮

which are also written in the form of linear algebraic equations as

$$\hat{f}_i^{(1)}-\sum_{j=1}^{15}E_j\hat{f}_j^{(1)}-3\hat{\mathbf{c}}_i\cdot\sum_{j=1}^{15}E_j\hat{\mathbf{c}}_j\hat{f}_j^{(1)}=0, \tag{2.2.29}$$

$$\hat{f}_i^{(m)}-\sum_{j=1}^{15}E_j\hat{f}_j^{(m)}-3\hat{\mathbf{c}}_i\cdot\sum_{j=1}^{15}E_j\hat{\mathbf{c}}_j\hat{f}_j^{(m)}=Ih_i^{(m)} \quad (m\geq 2), \tag{2.2.30}$$

where  $Ih_i^{(m)}$  represents the inhomogeneous terms given by

$$Ih_i^{(2)}=\frac{9}{2}(\hat{\mathbf{c}}_i\cdot\hat{\mathbf{u}}^{(1)})^2-\frac{3}{2}\hat{\mathbf{u}}^{(1)}\cdot\hat{\mathbf{u}}^{(1)}-\frac{\tau\Delta x}{k}\hat{\mathbf{c}}_i\cdot\hat{\nabla}\hat{f}_i^{(1)}, \tag{2.2.31a}$$

$$\begin{aligned}
Ih_i^{(3)} &= \frac{9}{2}\rho^{(1)}(\mathbf{c}_i\cdot\mathbf{u}^{(1)})^2+9(\mathbf{c}_i\cdot\mathbf{u}^{(1)})(\mathbf{c}_i\cdot\mathbf{u}^{(2)}) \\
& -\frac{3}{2}\rho^{(1)}\hat{\mathbf{u}}^{(1)}\cdot\hat{\mathbf{u}}^{(1)}-3\hat{\mathbf{u}}^{(1)}\cdot\hat{\mathbf{u}}^{(2)} \\
& -\frac{\tau\Delta x}{k}\hat{\mathbf{c}}_i\cdot\hat{\nabla}\hat{f}_i^{(2)}-\frac{\tau\Delta x}{k}\left[\frac{\text{Sh}}{k}\frac{\partial}{\partial t}+\frac{1}{2}\left(\frac{\Delta x}{k}\right)(\hat{\mathbf{c}}_i\cdot\hat{\nabla})^2\right]\hat{f}_i^{(1)} \\
& -\hat{\rho}^{(1)}(\hat{f}_i^{(2)}-\hat{f}_i^{\text{eq}(2)}), \tag{2.2.31b}
\end{aligned}$$

$$\begin{aligned}
Ih_i^{(1)} &= \frac{9}{2}\rho^{(2)}(\hat{\mathbf{c}}_i\cdot\hat{\mathbf{u}}^{(1)})^2+9\rho^{(1)}(\mathbf{c}_i\cdot\mathbf{u}^{(1)})(\hat{\mathbf{c}}_i\cdot\mathbf{u}^{(2)}) \\
& +\frac{9}{2}(\hat{\mathbf{c}}_i\cdot\hat{\mathbf{u}}^{(2)})^2+9(\hat{\mathbf{c}}_i\cdot\hat{\mathbf{u}}^{(1)})(\mathbf{c}_i\cdot\mathbf{u}^{(3)}) \\
& -\frac{3}{2}\rho^{(2)}\hat{\mathbf{u}}^{(1)}\cdot\hat{\mathbf{u}}^{(1)}-3\rho^{(1)}\hat{\mathbf{u}}^{(1)}\cdot\hat{\mathbf{u}}^{(2)}-\frac{3}{2}\hat{\mathbf{u}}^{(2)}\cdot\hat{\mathbf{u}}^{(2)}-3\hat{\mathbf{u}}^{(1)}\cdot\hat{\mathbf{u}}^{(3)} \\
& -\frac{\tau\Delta x}{k}\hat{\mathbf{c}}_i\cdot\hat{\nabla}\hat{f}_i^{(3)}-\frac{\tau\Delta x}{k}\left[\frac{\text{Sh}}{k}\frac{\partial}{\partial t}+\frac{1}{2}\left(\frac{\Delta x}{k}\right)(\hat{\mathbf{c}}_i\cdot\hat{\nabla})^2\right]\hat{f}_i^{(2)} \\
& -\left(\frac{\tau\Delta x}{k}\right)^2(\hat{\mathbf{c}}_i\cdot\hat{\nabla})\left[\frac{\text{Sh}}{k}\frac{\partial}{\partial t}+\frac{1}{6}\left(\frac{\Delta x}{k}\right)(\mathbf{c}_i\cdot\hat{\nabla})^2\right]\hat{f}_i^{(1)} \\
& -\hat{\rho}^{(1)}(\hat{f}_i^{(3)}-\hat{f}_i^{\text{eq}(3)})-\hat{\rho}^{(2)}(\hat{f}_i^{(2)}-\hat{f}_i^{\text{eq}(2)}). \tag{2.2.31c}
\end{aligned}$$

⋮

Equation (2.2.29) is a homogeneous linear algebraic equation and the solution is written with macroscopic variables by Equation (2.2.25) with Equation (2.2.24a).

Substituting Equation (2.2.25) into Equation (2.2.20c) we obtain

$$e^{(1)}=0, \tag{2.2.32}$$

Equation (2.2.30) are inhomogeneous linear algebraic equations for  $\hat{f}_i^{(m)}$  and have the same coefficient matrix in spite of  $m$  (see Appendix A). Thus, from the fundamental theorem of the linear algebra (Courant & Hilbert 1953; Strang 1976; see Appendix B) the solvability conditions for Equation (2.2.30) are obtained as follows:

$$\sum_{i=1}^{15}E_iIh_i^{(m)}=0 \quad (m\geq 2), \tag{2.2.33a}$$

$$\sum_{i=1}^{15}E_i\hat{\mathbf{c}}_{i\alpha}Ih_i^{(m)}=0 \quad (m\geq 2) \tag{2.2.33b}$$

with  $\alpha=1, 2, 3$ .

From the solvability conditions (2.2.33a) and (2.2.33b) for  $m = 2$ , we get the following partial differential equations for the component functions of the expansions of the macroscopic variables:

$$\frac{\partial \hat{u}_\alpha^{(1)}}{\partial \hat{x}_\alpha} = 0, \quad (2.2.34)$$

$$\frac{\partial \hat{\rho}^{(1)}}{\partial \hat{x}_\alpha} = 0 \quad (2.2.35)$$

with  $\alpha = 1, 2, 3$ . The summation convention is used for the subscript  $\alpha$  and  $\beta$  hereafter. Also, substituting Equation (2.2.26) into Equation (2.2.21c) we obtain

$$\hat{e}^{(2)} = 0, \quad (2.2.36)$$

From the solvability conditions (2.2.33a) and (2.2.33b) for  $m = 3$  we get

$$\frac{\text{Sh}}{k} \frac{\partial \hat{\rho}^{(1)}}{\partial \hat{t}} + \frac{\partial \hat{u}_\alpha^{(2)}}{\partial \hat{x}_\alpha} = 0, \quad (2.2.37)$$

$$\frac{\text{Sh}}{k} \frac{\partial \hat{u}_\alpha^{(1)}}{\partial \hat{t}} + \hat{u}_\beta^{(1)} \frac{\partial \hat{u}_\alpha^{(1)}}{\partial \hat{x}_\beta} = -\frac{1}{3} \frac{\partial \hat{\rho}^{(2)}}{\partial \hat{x}_\alpha} + \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{\Delta \hat{x}}{k} \frac{\partial^2 \hat{u}_\alpha^{(1)}}{\partial \hat{x}_\beta^2} \quad (2.2.38)$$

with  $\alpha, \beta = 1, 2, 3$ . Also, substituting Equation (2.2.27) into Equation (2.2.22c) we obtain

$$\hat{e}^{(3)} = -\frac{1}{3} \frac{\partial \hat{u}_\alpha^{(2)}}{\partial \hat{x}_\alpha}. \quad (2.2.39)$$

From the solvability conditions (2.2.33a) and (2.2.33b) for  $m = 4$  we get

$$\frac{\text{Sh}}{k} \frac{\partial \hat{\rho}^{(2)}}{\partial \hat{t}} + \frac{1}{6} \frac{\Delta \hat{x}}{k} \frac{\partial^2 \hat{\rho}^{(2)}}{\partial \hat{x}_\alpha^2} + \frac{\partial}{\partial \hat{x}_\alpha} (\rho^{(1)} \hat{u}_\alpha^{(2)} + \hat{\rho}^{(2)} \hat{u}_\alpha^{(1)} + \hat{u}_\alpha^{(3)}) = 0, \quad (2.2.40)$$

$$\begin{aligned} & \frac{\text{Sh}}{k} \frac{\partial}{\partial \hat{t}} (\hat{\rho}^{(1)} \hat{u}_\alpha^{(1)} + \hat{u}_\alpha^{(2)}) + \frac{\partial}{\partial \hat{x}_\beta} (\rho^{(1)} \hat{u}_\alpha^{(1)} \hat{u}_\beta^{(1)} + \hat{u}_\alpha^{(1)} \hat{u}_\beta^{(2)} + \hat{u}_\beta^{(1)} \hat{u}_\alpha^{(2)}) \\ &= -\frac{1}{3} \frac{\partial \hat{\rho}^{(3)}}{\partial \hat{x}_\alpha} + \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{\Delta \hat{x}}{k} \frac{\partial}{\partial \hat{x}_\beta} \left( \frac{\partial \hat{u}_\beta^{(2)}}{\partial \hat{x}_\alpha} + \frac{\partial \hat{u}_\alpha^{(2)}}{\partial \hat{x}_\beta} \right) \end{aligned} \quad (2.2.41)$$

with  $\alpha, \beta = 1, 2, 3$ .

From Equation (2.2.35) we get  $\hat{\rho}^{(1)} = C$  where  $C$  is a constant, if a boundary condition for  $\hat{\rho}^{(1)}$  is time-independent. Then, including the constant density in a reference density  $\rho_0$ , we can reduce to  $\hat{\rho}^{(1)} = 0$ . Hence, we obtain the governing equations for  $\hat{u}_\alpha^{(1)}$  and  $\hat{p}^{(2)}$ :

$$\frac{\partial \hat{u}_\alpha^{(1)}}{\partial \hat{x}_\alpha} = 0, \quad (2.2.42)$$

$$\frac{\text{Sh}}{k} \frac{\partial \hat{u}_\alpha^{(1)}}{\partial \hat{t}} + \hat{u}_\beta^{(1)} \frac{\partial \hat{u}_\alpha^{(1)}}{\partial \hat{x}_\beta} = -\frac{\partial \hat{p}^{(2)}}{\partial \hat{x}_\alpha} + \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{\Delta \hat{x}}{k} \frac{\partial^2 \hat{u}_\alpha^{(1)}}{\partial \hat{x}_\beta^2}, \quad (2.2.43)$$

and for  $\hat{u}_\alpha^{(2)}$  and  $\hat{p}^{(3)}$  we obtain

$$\frac{\partial \hat{u}_\alpha^{(2)}}{\partial \hat{x}_\alpha} = 0, \quad (2.2.44)$$

$$\frac{\text{Sh}}{k} \frac{\partial \hat{u}_\alpha^{(2)}}{\partial \hat{t}} + \hat{u}_\beta^{(1)} \frac{\partial \hat{u}_\alpha^{(2)}}{\partial \hat{x}_\beta} + \hat{u}_\beta^{(2)} \frac{\partial \hat{u}_\alpha^{(1)}}{\partial \hat{x}_\beta} = -\frac{\partial \hat{p}^{(3)}}{\partial \hat{x}_\alpha} + \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{\Delta \hat{x}}{k} \frac{\partial^2 \hat{u}_\alpha^{(2)}}{\partial \hat{x}_\beta^2}. \quad (2.2.45)$$

Multiplying Equation (2.2.42) by  $k$  and Equation (2.2.44) by  $k^2$  and taking the summation of both equations, we obtain

$$\frac{\partial}{\partial \hat{x}_\alpha} (k \hat{u}_\alpha^{(1)} + k^2 \hat{u}_\alpha^{(2)}) = 0, \quad (2.2.46)$$

and similarly, multiplying Equation (2.2.43) by  $k^2$  and Equation (2.2.45) by  $k^3$  and taking the summation of both equations, we obtain

$$\begin{aligned} & \text{Sh} \frac{\partial}{\partial t} (k \tilde{u}_\alpha^{(1)} + k^2 \tilde{u}_\alpha^{(2)}) + k \tilde{u}_\beta^{(1)} \frac{\partial}{\partial x_\beta} (k \tilde{u}_\alpha^{(1)} + k^2 \tilde{u}_\alpha^{(2)}) + k^2 \tilde{u}_\beta^{(2)} \frac{\partial}{\partial x_\beta} (k \tilde{u}_\alpha^{(1)}) \\ &= - \frac{\partial}{\partial x_\alpha} (k^2 p^{(2)} + k^3 p^{(3)}) \\ & \quad + \frac{1}{3} \left( \tau - \frac{1}{2} \right) \Delta \hat{x} \frac{\partial^2}{\partial x_\beta^2} (k \tilde{u}_\alpha^{(1)} + k^2 \tilde{u}_\alpha^{(2)}). \end{aligned} \quad (2.2.47)$$

Substituting  $k \tilde{u}_\alpha^{(1)} + k^2 \tilde{u}_\alpha^{(2)} + \delta_\alpha$  and  $k^2 p^{(2)} + k^3 p^{(3)} + \lambda$  into the continuity equation and the Navier-Stokes equations for incompressible fluid and comparing with Equations (2.2.46) and (2.2.47), we obtain the equations for  $\delta_\alpha$  and  $\lambda$  which are the same as the continuity equation and the Navier-Stokes equations with inhomogeneous terms of  $O(k^4)$ . From the equations for  $\delta_\alpha$  and  $\lambda$  it is seen that  $\delta_\alpha$  is of  $O(k^3)$  and  $\lambda$  is of  $O(k^4)$ . Hence, we find that  $k \tilde{u}_\alpha^{(1)} + k^2 \tilde{u}_\alpha^{(2)}$  and  $k^2 p^{(2)} + k^3 p^{(3)}$  are the solutions of the continuity equation and the Navier-Stokes equations for incompressible fluid with the errors of  $O(k^3)$  for velocities and  $O(k^4)$  for pressure gradient.

From higher-order solvability conditions we obtain similar equations for higher-order components of the macroscopic variables, but the equations are not the same as the continuity equation and the Navier-Stokes equations for incompressible fluid for the higher-order components. Therefore, it follows that by using Equation (2.2.13) with Equations (2.2.7)–(2.2.10) and (2.2.12) we can obtain the macroscopic flow velocities and the pressure gradient for incompressible fluid with relative errors of  $O(k^2)$ .

In addition, it is found from Equation (2.2.47) that the viscosity of the fluid is given in the dimensionless form as follows:

$$\mu = \frac{\mu}{\rho_0 c L} = \frac{1}{3} \left( \tau - \frac{1}{2} \right) \Delta \hat{x}. \quad (2.2.48)$$

Thus, we obtain the following relation in general:

$$\text{Ma} = \frac{1}{3} \left( \tau - \frac{1}{2} \right) \Delta \hat{x} \text{Re}. \quad (2.2.49)$$

Taking account of the relation of Equation (2.2.49), we see that the relative errors of Equations (2.2.13) with Equations (2.2.7)–(2.2.10) and (2.2.12) against the continuity equation and the Navier-Stokes equations for incompressible fluid are of  $O(\text{Ma}^2)$  for a fixed Reynolds number and they do not change for fixed Reynolds and Mach numbers. Finally, it is noted that in practical calculations of incompressible fluid flows by LBM, we first specify the value of Re and then choose the values of  $\Delta \hat{x}$  and  $\tau$  so that  $\text{Ma} = O(\Delta \hat{x})$  using the relation of Equation (2.2.49) and considering that relative errors become  $O(k^2)$ .

## 2.3 Boundary Conditions in the LBM

### 2.3.1 No-slip Boundary Condition at Wall

First, a new approach for applying a no-slip boundary condition at a wall is presented. For explanation the fifteen-velocity model is used, but it is straightforward to apply the method to other velocity models. Also, we use the horizontal wall shown in Figure 2.2 to explain the procedure of the method, but it is easy to extend the method to the inclined wall (see Chapter 3).

Hereafter, non-dimensional variables are used as in Section 2.2.1 and the caret symbol denoting non-dimensional properties is not written for the sake of simplicity. At the no-slip wall we have to specify the distribution functions whose velocity points

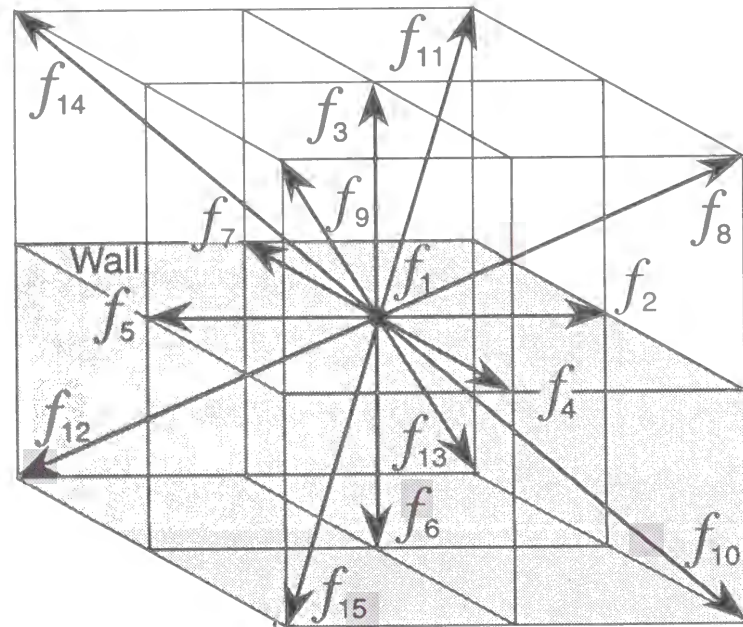


Figure 2.2: Particle distribution functions of the fifteen-velocity model at the wall.

to fluid region. In Figure 2.2, for example, the unknown distribution functions are  $f_3$ ,  $f_8$ ,  $f_9$ ,  $f_{11}$ , and  $f_{14}$ . In the kinetic theory of gases the assumption of diffuse reflection is often used at the wall. In this approximation gas molecules that strike the wall are assumed to leave it with a Maxwellian velocity distribution having the velocity and the temperature of the wall (Sone & Aoki 1994). In general, the velocity along the wall obtained with this assumption is not equal to that of the wall velocity, although the normal velocity to the wall is equal to that of the wall velocity. The difference between the fictitious velocity and the wall velocity is called the slip velocity. The idea of the present method is that the unknown distribution functions are assumed to be the equilibrium distribution functions with a counter slip velocity which is determined so that the fluid velocity at the wall is equal to the wall velocity. That is, in the case of Figure 2.2 the unknown distribution functions  $f_3$ ,  $f_8$ ,  $f_9$ ,  $f_{11}$ , and  $f_{14}$  are assumed to be

$$f_i = E_i \rho' \left\{ 1 + 3(u_0 + v_w + w_0) + \frac{9}{2}(u_0 + v_w + w_0)^2 - \frac{3}{2}[(u_w + u')^2 + v_w^2 + (w_w + w')^2] \right\} \quad \text{for } i = 3, 8, 9, 11, 14, \quad (2.3.1)$$

where

$$\left. \begin{aligned} u_0 &= 0, & w_0 &= 0 & \text{for } i &= 3, \\ u_0 &= u_w + u', & w_0 &= w_w + w' & \text{for } i &= 8, \\ u_0 &= -u_w - u', & w_0 &= w_w + w' & \text{for } i &= 9, \\ u_0 &= u_w + u', & w_0 &= -w_w - w' & \text{for } i &= 11, \\ u_0 &= -u_w - u', & w_0 &= -w_w - w' & \text{for } i &= 14, \end{aligned} \right\} \quad (2.3.2)$$

where  $u_w$ ,  $v_w$ , and  $w_w$  are the  $x$ -,  $y$ -, and  $z$ -components of the wall velocity, respectively, and  $\rho'$ ,  $u'$ , and  $w'$  are unknown parameters. The unknown  $u'$  and  $w'$  are the

two components of the above-mentioned counter slip velocity. It is noted that we have no normal velocity jump at the wall because as mentioned above there exists no difference of the normal velocity to the wall between the fluid and the wall on the assumption of diffuse reflection. The three unknown parameters are determined on the condition that the fluid velocity at the wall is equal to the wall velocity. Hence, we obtain three equations corresponding to the  $x$ -,  $y$ -, and  $z$ -components of the fluid velocity. Moreover, the density at the wall,  $\rho_w$ , is an unknown quantity and is calculated by Equation (2.2.7). Therefore, we finally obtain four equations for the four unknowns. The solutions are as follows:

$$\rho_w = \frac{1}{1 - v_w} \left[ f_1 + f_2 + f_4 + f_5 + f_7 + 2(f_6 + f_{10} + f_{12} + f_{13} + f_{15}) \right]. \quad (2.3.3)$$

$$\rho' = 6 \frac{\rho_w v_w + (f_6 + f_{10} + f_{12} + f_{13} + f_{15})}{1 + 3v_w + 3v_w^2}. \quad (2.3.4)$$

$$u' = \frac{1}{1 + 3v_w} \left[ 6 \frac{\rho_w u_w - (f_2 - f_5 + f_{10} - f_{12} + f_{13} - f_{15})}{\rho'} - u_w - 3u_w v_w \right]. \quad (2.3.5)$$

$$w' = \frac{1}{1 + 3v_w} \left[ 6 \frac{\rho_w w_w - (f_1 - f_7 + f_{10} - f_{12} - f_{13} + f_{15})}{\rho'} - w_w - 3v_w w_w \right]. \quad (2.3.6)$$

Substituting Equations (2.3.4)-(2.3.6) into Equation (2.3.1), all the unknown distribution functions at the wall are determined.

### 2.3.2 Periodic Boundary Condition at Inlet and Outlet

A periodic boundary condition with a pressure difference  $\Delta p$  at the inlet and outlet is presented. Hereafter, the subscript 'in' and 'out' represent quantities at the inlet and outlet, respectively. Figure 2.3 shows the distribution functions at the inlet and outlet. At the inlet in Figure 2.3(a), the unknown distribution functions are  $f_2$ ,  $f_8$ ,  $f_{10}$ ,  $f_{11}$ , and  $f_{13}$ . Taking account of the form of the equilibrium distribution functions given by Equation (2.2.12) and neglecting the second- and higher-order terms of Knudsen number compared with the terms of  $O(1)$ , it is assumed that the unknown distribution functions at the inlet can be written by adding constant values  $K$  and  $K/8$  to the corresponding known distribution functions at the outlet:

$$f_2|_{\text{in}} = f_2|_{\text{out}} + K. \quad (2.3.7)$$

$$f_i|_{\text{in}} = f_i|_{\text{out}} + \frac{1}{8}K \quad \text{for } i = 8, 10, 11, 13. \quad (2.3.8)$$

Similarly, at the outlet in Figure 2.3(b), the unknown distribution functions  $f_5$ ,  $f_9$ ,  $f_{12}$ ,  $f_{14}$ , and  $f_{15}$  are assumed to be written by subtracting the constant values from the corresponding known distribution functions at the inlet:

$$f_5|_{\text{out}} = f_5|_{\text{in}} - K. \quad (2.3.9)$$

$$f_i|_{\text{out}} = f_i|_{\text{in}} - \frac{1}{8}K \quad \text{for } i = 9, 12, 14, 15. \quad (2.3.10)$$

Then the constant value  $K$  is determined so that the pressure difference between the inlet and outlet is equal to  $\Delta p$ . That is, using Equations (2.2.7), (2.2.9), and (2.2.10), we get

$$K = \Delta p - \frac{1}{3} (f_1|_{\text{in}} - f_1|_{\text{out}} + f_3|_{\text{in}} - f_3|_{\text{out}} + f_4|_{\text{in}} - f_4|_{\text{out}} + f_6|_{\text{in}} - f_6|_{\text{out}} + f_7|_{\text{in}} - f_7|_{\text{out}}). \quad (2.3.11)$$

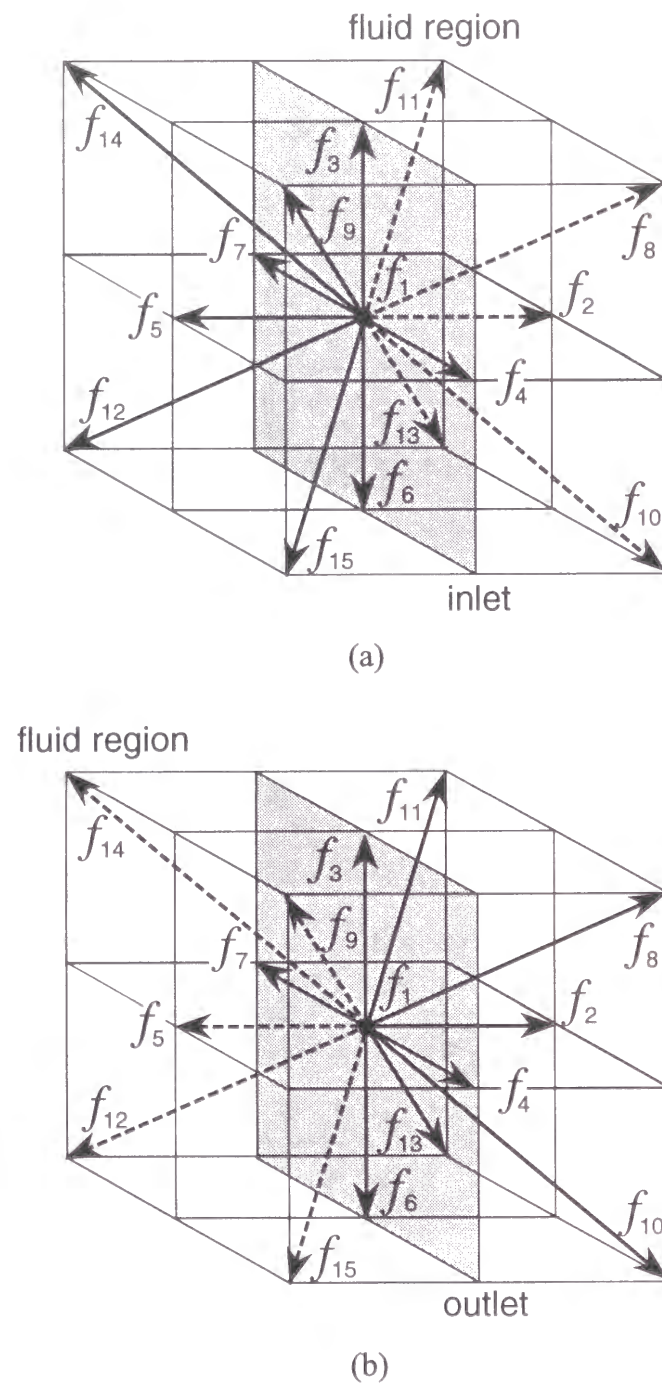


Figure 2.3: Particle distribution functions of the fifteen-velocity model: (a) at the inlet; (b) at the outlet. The solid and dashed arrows indicate the known and unknown distribution functions, respectively.

Substituting Equation (2.3.11) into Equations (2.3.7)–(2.3.10), all the unknown distribution functions at the inlet and outlet are determined for the given  $\Delta p$ .

In addition, on the corner lines of the inlet and outlet the unknown distribution functions are calculated by combining the above-mentioned periodic and no-slip boundary conditions as follows. For example, on the bottom lines of the inlet and outlet in Figure 2.3, we first express the unknown distribution functions  $f_2|_{\text{in}}$ ,  $f_{10}|_{\text{in}}$ ,  $f_{13}|_{\text{in}}$ ,  $f_5|_{\text{out}}$ ,  $f_{12}|_{\text{out}}$ , and  $f_{15}|_{\text{out}}$  by using Equations (2.3.7)–(2.3.10) with a constant value  $K_0$ . Then, applying the no-slip boundary conditions on the lines and specifying the pressure difference between the inlet and outlet, we obtain nine equations for nine unknowns. The solution for  $K_0$  is given by

$$K_0 = \Delta p(1 - v_w) - \frac{1}{3}[f_1|_{\text{in}} - f_1|_{\text{out}} + f_4|_{\text{in}} - f_4|_{\text{out}} + f_7|_{\text{in}} - f_7|_{\text{out}} + 2(f_6|_{\text{in}} - f_6|_{\text{out}})]. \quad (2.3.12)$$

The solutions of the other unknowns can also be obtained by using Equations (2.3.3)–(2.3.6). Thus, the unknown distribution functions are determined by Equations (2.3.1) and (2.3.7)–(2.3.10).

## 2.4 LBM for Binary Fluid Mixture

### 2.4.1 Basic Equation

In the following, the LBM for a binary fluid mixture with a simple kinetic model is proposed to simulate flow and mass transfer problems. Here, it is assumed that an isothermal binary fluid mixture of  $A$ - and  $B$ -species under the condition that the fraction of  $B$ -species is much smaller than that of  $A$ -species. Under this condition, the effect of  $A$ – $B$  collisions can be neglected compared to  $A$ – $A$  collisions. Also,

the effect of  $B$ - $B$  collisions can be neglected in comparison with  $B$ - $A$  collisions. Therefore, the evolution equation of the particle distribution function  $f_{\sigma i}$  of  $\sigma$ -species ( $\sigma = A, B$ ) with velocity  $\mathbf{c}_i$  ( $i = 1, 2, 3, \dots, 15$ ) at the point  $\mathbf{x}$  and time  $t$  can be written as follows:

$$f_{\sigma i}(\mathbf{x} + \mathbf{c}_i \Delta x, t + \Delta t) - f_{\sigma i}(\mathbf{x}, t) = -\frac{1}{\tau_\sigma} [f_{\sigma i}(\mathbf{x}, t) - f_{\sigma Ai}^{\text{eq}}(\mathbf{x}, t)]$$

$$\text{for } i = 1, 2, 3, \dots, 15, \quad \sigma = A, B. \quad (2.4.1)$$

where  $f_{\sigma Ai}^{\text{eq}}$  is an equilibrium distribution function for  $\sigma$ -species and  $\tau_\sigma$  is a single relaxation time of  $O(1)$ .

As in the kinetic theory of gases, we define the density  $\rho_A$  of component  $A$ , the concentration  $\rho_B$  of component  $B$ , the flow velocity  $\mathbf{u}_\sigma$  of component  $\sigma$  ( $\sigma = A, B$ ), and the internal energy  $e_A$  of component  $A$  in terms of the particle distribution function as follows:

$$\rho_\sigma = \sum_{i=1}^{15} f_{\sigma i} \quad \text{for } \sigma = A, B. \quad (2.4.2)$$

$$\mathbf{u}_\sigma = \frac{1}{\rho_\sigma} \sum_{i=1}^{15} f_{\sigma i} \mathbf{c}_i \quad \text{for } \sigma = A, B. \quad (2.4.3)$$

$$e_A = \frac{1}{2\rho_A} \sum_{i=1}^{15} f_{Ai} (\mathbf{c}_i - \mathbf{u}_A) \cdot (\mathbf{c}_i - \mathbf{u}_A), \quad (2.4.4)$$

and also we define pressure  $p_A$  of component  $A$  by

$$p_A = \frac{2}{3} \rho_A e_A. \quad (2.4.5)$$

Here, it should be noted that Equation (2.4.1) for component  $A$  has the same form as Equation (2.2.13) for single phase flow. Thus, the equilibrium distribution function

$f_{Ai}^{\text{eq}}$  is also the same as Equation (2.2.12), i.e.,

$$f_{Ai}^{\text{eq}} = E_i \rho_A \left[ 1 + 3\mathbf{c}_i \cdot \mathbf{u}_A + \frac{9}{2} (\mathbf{c}_i \cdot \mathbf{u}_A)^2 - \frac{3}{2} \mathbf{u}_A \cdot \mathbf{u}_A \right] \quad \text{for } i = 1, 2, 3, \dots, 15. \quad (2.4.6)$$

On the other hand, we proposed a new equilibrium distribution function  $f_{BAi}^{\text{eq}}$  as follows. We referred to the kinetic model for a multicomponent gas proposed by Garzó, Santos & Brey (1992) and assumed the following form of equilibrium distribution function:

$$f_{BAi}^{\text{eq}} = E_i \rho_B \left[ 1 + 3\mathbf{c}_i \cdot \mathbf{u}_A + \frac{9}{2} (\mathbf{c}_i \cdot \mathbf{u}_A)^2 - \frac{3}{2} \mathbf{u}_A \cdot \mathbf{u}_A \right]$$

$$\times \left[ 1 + \lambda_1 (\mathbf{u}_B - \mathbf{u}_A) \cdot (\mathbf{u}_B - \mathbf{u}_A) + \lambda_2 (\mathbf{u}_B - \mathbf{u}_A) \cdot (\mathbf{c}_i - \mathbf{u}_A) \right.$$

$$\left. + \lambda_3 (\mathbf{u}_B - \mathbf{u}_A) \cdot (\mathbf{u}_B - \mathbf{u}_A) (\mathbf{c}_i - \mathbf{u}_A) \cdot (\mathbf{c}_i - \mathbf{u}_A) \right], \quad (2.4.7)$$

where  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  are unknown parameters. These three parameters are determined so that total mass, total momentum, and total energy of  $B$ -species are conserved in the collision at each lattice node. That is,

$$\sum_{i=1}^{15} (f_{Bi} - f_{BAi}^{\text{eq}}) = 0, \quad (2.4.8a)$$

$$\sum_{i=1}^{15} \mathbf{c}_i (f_{Bi} - f_{BAi}^{\text{eq}}) = 0, \quad (2.4.8b)$$

$$\frac{1}{2} \sum_{i=1}^{15} (\mathbf{c}_i - \mathbf{u}_B) \cdot (\mathbf{c}_i - \mathbf{u}_B) (f_{Bi} - f_{BAi}^{\text{eq}}) = 0. \quad (2.4.8c)$$

Consequently, we obtain

$$\lambda_1 = -\frac{3}{4}, \quad \lambda_2 = \frac{3}{2}, \quad \lambda_3 = \frac{3}{4}. \quad (2.4.9)$$

In practice, only the terms up to  $O(u)$  in Equation (2.4.7) are taken into account, because the convection-diffusion equation contains no terms of second order in velocity, although the terms up to  $O(u^2)$  are required to obtain the convection term in the Navier-Stokes equations (Rothman & Zaleski 1997). Therefore, the resulting equilibrium distribution function  $f_{Bi}^{eq}$  is reduced to

$$f_{Bi}^{eq} = E_i \rho_B \left[ 1 + \frac{3}{2} \mathbf{c}_i \cdot (\mathbf{u}_A + \mathbf{u}_B) \right] \quad \text{for } i = 1, 2, 3, \dots, 15. \quad (2.4.10)$$

### 2.4.2 Fluid-Dynamic Type Equation

Fluid-dynamic type equations are derived by using the S-expansion procedure of the asymptotic theory in Section 2.2.2. Here is also considered the case of a small Knudsen number with finite Reynolds number. In this case, since Mach number is regarded as the same order as Knudsen number, it is assumed that the deviation of the distribution function from its equilibrium state at rest with the local density is of the same order as Knudsen number. Then  $f_{Ai}$  and  $f_{Bi}$  are expanded as follows:

$$f_{\sigma i} = E_i (\rho_\sigma^{(0)} + k f_{\sigma i}^{(1)} + k^2 f_{\sigma i}^{(2)} + k^3 f_{\sigma i}^{(3)} + k^4 f_{\sigma i}^{(4)} + \dots) \quad \text{for } i = 1, 2, 3, \dots, 15, \quad \sigma = A, B. \quad (2.4.11)$$

where  $\rho_A^{(0)} = 1$ , and  $k = O(\Delta x)$  is of the same order as Knudsen number and is related to  $\tau_\sigma$ . Corresponding to Equation (2.4.11), the macroscopic variables are also expanded as follows:

$$\rho_\sigma = \rho_\sigma^{(0)} + k \rho_\sigma^{(1)} + k^2 \rho_\sigma^{(2)} + k^3 \rho_\sigma^{(3)} + \dots \quad \text{for } \sigma = A, B. \quad (2.4.12)$$

$$\mathbf{u}_\sigma = k \mathbf{u}_\sigma^{(1)} + k^2 \mathbf{u}_\sigma^{(2)} + k^3 \mathbf{u}_\sigma^{(3)} + \dots \quad \text{for } \sigma = A, B. \quad (2.4.13)$$

$$c_A = \frac{1}{2} + k c_A^{(1)} + k^2 c_A^{(2)} + k^3 c_A^{(3)} + \dots, \quad (2.4.14)$$

$$p_A = \frac{1}{3} + k p_A^{(1)} + k^2 p_A^{(2)} + k^3 p_A^{(3)} + \dots, \quad (2.4.15)$$

Also, the equilibrium distribution functions  $f_{\sigma i}^{eq}$  are expanded as follows:

$$f_{\sigma i}^{eq} = E_i (\rho_\sigma^{(0)} + k f_{\sigma i}^{eq(1)} + k^2 f_{\sigma i}^{eq(2)} + k^3 f_{\sigma i}^{eq(3)} + k^4 f_{\sigma i}^{eq(4)} + \dots) \quad \text{for } i = 1, 2, 3, \dots, 15, \quad \sigma = A, B. \quad (2.4.16)$$

Substituting these equations into Equation (2.4.1), we obtain inhomogeneous linear algebraic equations for the component functions  $f_{\sigma i}^{(m)}$  ( $m = 1, 2, 3, \dots$ ). From the solvability conditions in the fundamental theorem of the linear algebra, it is shown that  $\mathbf{u}_A = k \mathbf{u}_A^{(1)} + k^2 \mathbf{u}_A^{(2)} + O(k^3)$  and  $p_A = k^2 p_A^{(2)} + k^3 p_A^{(3)} + O(k^4)$  satisfy

$$\frac{\partial u_{A\alpha}}{\partial x_\alpha} = 0, \quad (2.4.17)$$

$$\text{Sh} \frac{\partial u_{A\alpha}}{\partial t} + u_{A\beta} \frac{\partial u_{A\alpha}}{\partial x_\beta} = - \frac{\partial p_A}{\partial x_\alpha} + \frac{1}{3} \left( \tau_A - \frac{1}{2} \right) \Delta x \frac{\partial^2 u_{A\alpha}}{\partial x_\beta^2}, \quad (2.4.18)$$

and  $\rho_B = \rho_B^{(0)} + k \rho_B^{(1)} + O(k^2)$  satisfies

$$\text{Sh} \frac{\partial \rho_B}{\partial t} + u_{A\alpha} \frac{\partial \rho_B}{\partial x_\alpha} = \frac{2}{3} \left( \tau_B - \frac{1}{4} \right) \Delta x \frac{\partial^2 \rho_B}{\partial x_\alpha^2}, \quad (2.4.19)$$

where  $\alpha, \beta = 1, 2, 3$ . Equations (2.4.17) and (2.4.18) correspond to the continuity equation and the Navier-Stokes equations for incompressible fluid of component A, respectively. Also, Equation (2.4.19) corresponds to the convection-diffusion equation for component B in the binary fluid mixture. Therefore, it is found that

using Equations (2.4.1)–(2.4.6) for  $\sigma = A$ , we can obtain the flow velocities and the pressure gradient for incompressible fluid of component  $A$  with relative errors of  $O(k^2)$ . And it is also found that using Equations (2.4.1)–(2.4.3) and (2.4.10) for  $\sigma = B$  we can obtain the concentration of diffusing component  $B$  in a binary fluid mixture with relative errors of  $O(k^2)$ .

In addition, from Equations (2.4.18) and (2.4.19) the viscosity  $\mu$  of the fluid and the diffusivity  $D_{BA}$  in the binary fluid mixture are related to  $\tau_A$ ,  $\tau_B$ , and  $\Delta x$  as follows:

$$\mu = \frac{1}{3} \left( \tau_A - \frac{1}{2} \right) \Delta x, \quad (2.4.20)$$

$$D_{BA} = \frac{2}{3} \left( \tau_B - \frac{1}{4} \right) \Delta x. \quad (2.4.21)$$

### 2.4.3 Boundary Condition at Wall

Finally, we present boundary condition for component  $B$  at wall, which is needed in the following simulations. Here, the case that constant concentration of component  $B$  is given at the wall is considered. For example, at the wall in Figure 2.2, the unknown distributions are  $f_{B3}$ ,  $f_{B8}$ ,  $f_{B9}$ ,  $f_{B11}$ , and  $f_{B14}$ . As in the single phase flow, the unknown distribution functions are assumed to be the equilibrium distribution function given by Equation (2.4.10) with counter slip velocity having two components. The unknown distribution functions are given by

$$f_{Bi} = E_i \rho'_B \left[ 1 + \frac{3}{2} (u_{B0} + v_w + w_{B0}) \right] \quad \text{for } i = 3, 8, 9, 11, 14, \quad (2.4.22)$$

where

$$\left. \begin{aligned} u_{B0} &= 0, & w_{B0} &= 0 & \text{for } i &= 3, \\ u_{B0} &= u_w + u'_B, & w_{B0} &= u_w + u'_B & \text{for } i &= 8, \\ u_{B0} &= -u_w - u'_B, & w_{B0} &= u_w + u'_B & \text{for } i &= 9, \\ u_{B0} &= u_w + u'_B, & w_{B0} &= -u_w - u'_B & \text{for } i &= 11, \\ u_{B0} &= -u_w - u'_B, & w_{B0} &= -u_w - u'_B & \text{for } i &= 14, \end{aligned} \right\} \quad (2.4.23)$$

where  $\rho'_B$ ,  $u'_B$ , and  $w'_B$  are unknown parameters. The unknown  $u'_B$  and  $w'_B$  are two components of the counter slip velocity. The three unknown parameters are determined on the conditions that two components of the fluid velocity along the wall are equal to those of the wall velocity and that concentration of component  $B$  at the wall is equal to a given value  $\rho_B|_w$ . Thus, we obtain three equations for the three unknowns. The solutions are as follows:

$$\rho'_B = \frac{12}{2 + 3v_w} \left[ \rho_B|_w - (f_{B1} + f_{B2} + f_{B4} + f_{B5} + f_{B6} + f_{B7} + f_{B10} + f_{B12} + f_{B13} + f_{B15}) \right], \quad (2.4.24)$$

$$u'_B = 12 \frac{\rho_B|_w u_w - (f_{B2} + f_{B5} + f_{B10} + f_{B12} + f_{B13} + f_{B15})}{\rho'_B} - u_w, \quad (2.4.25)$$

$$w'_B = 12 \frac{\rho_B|_w w_w - (f_{B4} + f_{B7} + f_{B10} + f_{B12} + f_{B13} + f_{B15})}{\rho'_B} - w_w. \quad (2.4.26)$$

Substituting Equations (2.4.24)–(2.4.26) into Equation (2.4.22), all the unknown distribution functions for component  $B$  at the wall are determined.

## 2.5 Numerical Examples

To demonstrate the validity of the methods described in preceding Sections, two fundamental steady problems are calculated. The first problem is a three-

dimensional flow through a square duct with a constant pressure gradient. The second problem is a mass transfer between two parallel plates. In both simulations, the LBM with the fifteen-velocity model is used.

### 2.5.1 Flow through Square Duct

The first problem is a flow through a square duct whose sizes are at  $x_2 = \pm 1/2$  and  $x_3 = \pm 1/2$ . The non-dimensional  $x_1$ -momentum equation for this problem is

$$\frac{dp}{dx_1} = \mu \left( \frac{\partial^2 u_1}{\partial x_2^2} + \frac{\partial^2 u_1}{\partial x_3^2} \right). \quad (2.5.1)$$

The analytical solution  $u_1^*$  is given by

$$u_1^*(x_2, x_3) = -\frac{1}{2\mu} \frac{dp}{dx_1} \left[ \frac{1}{4} - x_2^2 + 8 \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell+1}}{n^3} \operatorname{sech} \frac{n}{2} \cosh nx_3 \cos nx_2 \right], \quad (2.5.2)$$

where  $n = (2\ell + 1)\pi$ .

In the LBM simulations, we maintain the conditions at  $\operatorname{Re} = u_{1,\max}^*/\mu = 2$ , where  $u_{1,\max}^*$  is the analytical velocity at  $x_2 = 0$  and  $x_3 = 0$ . On the walls and at the inlet and outlet we use the no-slip boundary condition and the periodic boundary condition with constant pressure gradient described in Section 2.3, respectively. It is noted that on four corner lines along  $x_1$ -direction and at every corner point of the walls, one cannot determine unknown distribution functions by using these boundary conditions, since there exist distribution functions whose velocity points from the outer to outer region. Thus, in the following calculations, all the distribution functions including known distribution functions at the nodes are set to be averaged value of the corresponding distribution function at two nearest neighboring lattice nodes in the  $x_2$ - and  $x_3$ -directions. The calculations are carried out with  $\Delta x = 1/10, 1/20$ , and  $1/30$  and with  $\tau = 0.8, 1.1$ , and  $1.4$ , while  $\operatorname{Re}$  is kept at the constant value of 2.

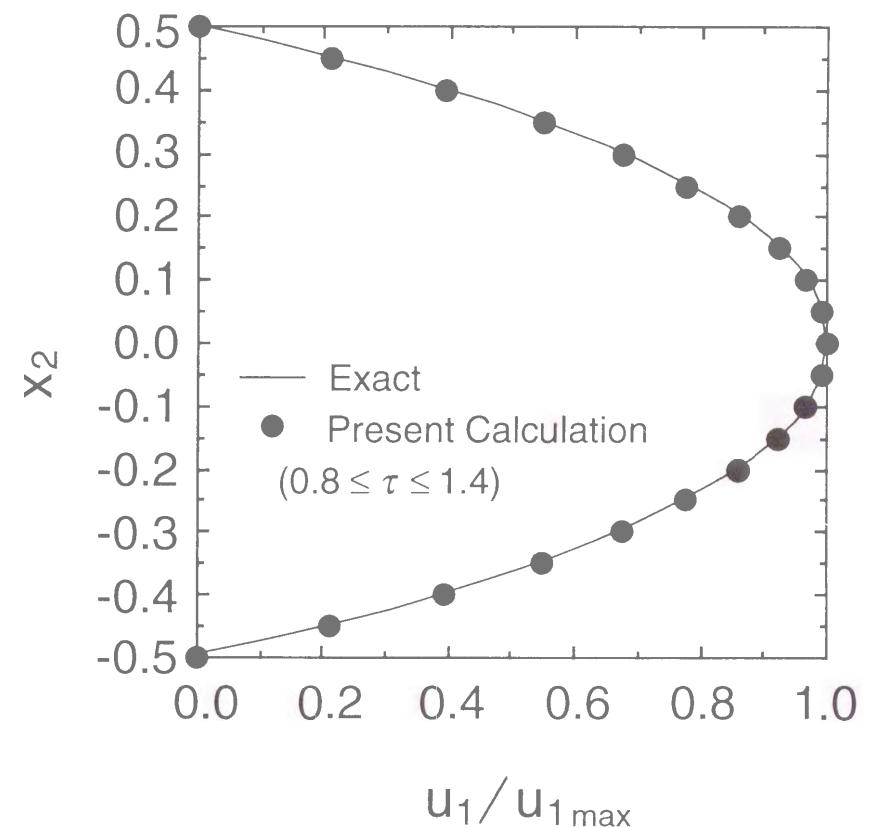


Figure 2.4: Calculated velocity profiles  $u_1/u_{1,\max}$  along the  $x_2$ -direction at  $x_3 = 0$  of a flow through square duct with  $\Delta x = 0.05$  and  $\tau = 0.8, 1.1$ , and  $1.4$ .

Table 2.1: Space-averaged values of counter slip velocity  $-\bar{u}'_1/u_{1,\max}$  at every wall in the calculations with the present boundary condition for different  $\tau$  and  $\Delta x$ .

|              | $\Delta x = 1/10$     | $\Delta x = 1/20$     | $\Delta x = 1/30$     |
|--------------|-----------------------|-----------------------|-----------------------|
| $\tau = 0.8$ | $3.29 \times 10^{-1}$ | $1.50 \times 10^{-1}$ | $9.67 \times 10^{-2}$ |
| $\tau = 1.1$ | $4.57 \times 10^{-1}$ | $2.10 \times 10^{-1}$ | $1.35 \times 10^{-1}$ |
| $\tau = 1.4$ | $5.86 \times 10^{-1}$ | $2.71 \times 10^{-1}$ | $1.70 \times 10^{-1}$ |

Figure 2.4 shows the calculated velocity profiles  $u_1/u_{1,\max}$  along  $x_2$ -direction at  $x_3 = 0$  with  $\Delta x = 0.05$  and  $\tau = 0.8, 1.1$ , and  $1.4$ . It is seen that the calculated results for  $0.8 \leq \tau < 1.4$  agree well with the analytical solution within machine accuracy. For different  $\tau$  and  $\Delta x$ , the space-averaged values of the counter slip velocity  $-\bar{u}'_1/u_{1,\max}$  at every wall are shown in Table 2.1. Note that the values of  $\bar{u}'_1$  are negative for all cases. It is found from the results that the magnitude of the counter slip velocity increases as  $\tau$  and  $\Delta x$  become larger. For comparison with the present results, the simulation of the same problem are carried out with the bounce-back boundary condition in which  $f_3 = f_6$ ,  $f_8 = f_{12}$ ,  $f_9 = f_{13}$ ,  $f_{11} = f_{15}$ , and  $f_{14} = f_{10}$ . For fixed  $\Delta x = 0.05$ , the calculated values of the slip velocity  $u_s$  are  $u_s/u_{1,\max} = 5.42 \times 10^{-3}$ ,  $1.46 \times 10^{-2}$ , and  $2.71 \times 10^{-2}$  with  $\tau = 0.8, 1.1$ , and  $1.4$ , respectively. It is found from the results that using the bounce-back boundary condition we have the slip velocity at the wall and the slip velocity increases as  $\tau$  becomes larger. Next, the errors of the calculated results from the analytical solution are examined for various  $\Delta x$  and  $\tau$ . If we take the ordering of the asymptotic theory into account, the left-hand side of Equation (2.5.1) is of  $O(k^2)$  since  $dp^{(1)}/dx_1 = 0$ , and the right-hand side is of  $O(\mu k)$ . It follows that  $k$  is of  $O(\mu)$  and hence the errors are proportional to  $[(\tau - \frac{1}{2})\Delta x]^2$ . Figure 2.5 shows the error norm  $Er_1 = \sum_{x_2} \sum_{x_3} |u_1 - u_1^*| / \sum_{x_2} \sum_{x_3} |u_1^*|$

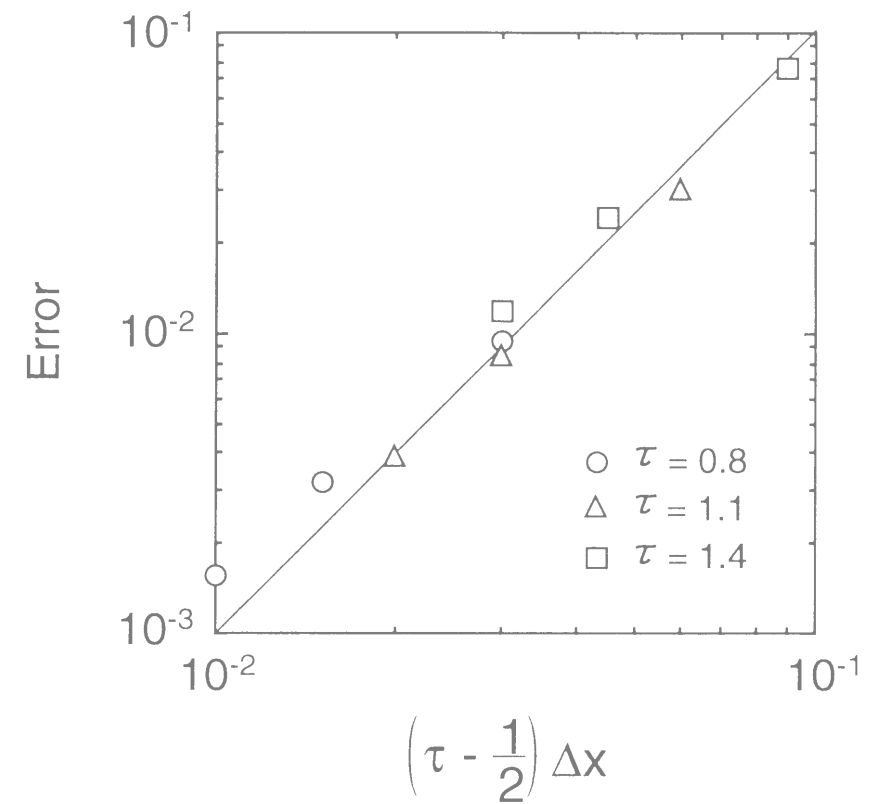


Figure 2.5: Error norm of a flow through a square duct. The solid line indicates an incline of 2.

where the sums are taken over the same  $11 \times 11$  nodes on the square section for all cases. It is found that the errors decrease almost in proportion to  $[(\tau - \frac{1}{2})\Delta x]^2$  for various combinations of  $\Delta x$  and  $\tau$ . The small dispersion of the errors at the same value of  $(\tau - \frac{1}{2})\Delta x$  is due to the incomplete implementation of boundary conditions such as periodic conditions with constant pressure gradient at inlet and outlet and no-slip conditions at corner lines on walls.

### 2.5.2 Diffusion Problem between Parallel Walls

The second problem is a mass transfer between two parallel walls. The lower and upper walls are located at  $x_2 = 0$  and  $x_2 = 1$ , respectively. The two walls are assumed porous ones and a constant normal flow  $v_{A0}$  of component  $A$  is injected through the lower wall and is removed from the upper wall. On the other hand, the concentration of component  $B$  at the lower and upper wall is maintained with  $\rho_{B0}$  and  $\rho_{B1}$  ( $\rho_{B0} < \rho_{B1}$ ), respectively. Therefore, component  $B$  diffuses counter to the flow of component  $A$ . The governing equation for this steady state problem becomes

$$v_{A0} \frac{d\Pi_B}{dx_2} = D_{BA} \frac{d^2\Pi_B}{dx_2^2}. \quad (2.5.3)$$

where  $\Pi_B$  is a dimensionless concentration defined as follows:

$$\Pi_B = \frac{\rho_B - \rho_{B0}}{\rho_{B1} - \rho_{B0}}. \quad (2.5.4)$$

The analytical solution  $\Pi_B^*$  is given by

$$\Pi_B^* = \frac{\exp(v_{A0}x_2/D_{BA}) - 1}{\exp(v_{A0}/D_{BA}) - 1}. \quad (2.5.5)$$

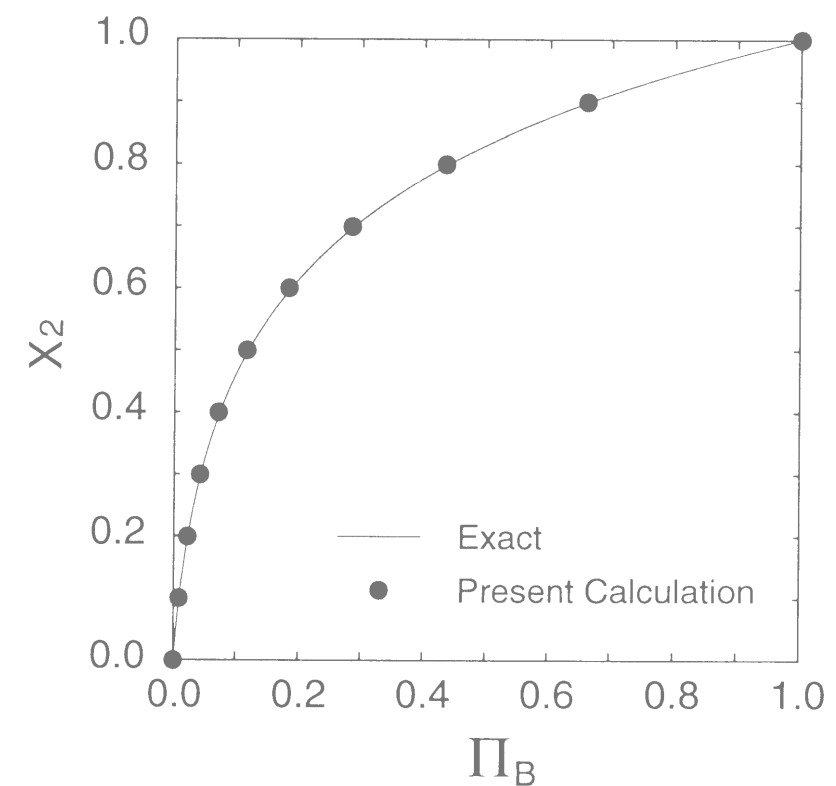


Figure 2.6: Calculated concentration profile  $\Pi_B = (\rho_B - \rho_{B0})/(\rho_{B1} - \rho_{B0})$  of a mass transfer problem between two parallel walls with  $\Delta x = 0.1$  and  $\tau_B = 0.85$ .

Table 2.2: Error norms of diffusion problem between parallel walls.

| $\Delta x$ | $\tau_B$             | $Er_1$                | $Er_2$                |
|------------|----------------------|-----------------------|-----------------------|
| 0.1        | 0.85, 1.15, and 1.45 | $8.13 \times 10^{-3}$ | $6.61 \times 10^{-3}$ |
| 0.05       | 0.85, 1.15, and 1.45 | $2.01 \times 10^{-3}$ | $1.63 \times 10^{-3}$ |
| 0.025      | 0.85, 1.15, and 1.45 | $5.00 \times 10^{-4}$ | $4.06 \times 10^{-4}$ |
| 0.0125     | 0.85, 1.15, and 1.45 | $1.25 \times 10^{-4}$ | $1.01 \times 10^{-4}$ |

In the following calculations, we maintain the conditions at  $v_{A0}/D_{BA} = 4$  and  $\rho_{B1} = \rho_{B0} = 1$ . The periodic boundary condition is imposed in the  $x_1$ - and  $x_3$ -directions. On the lower and upper walls the boundary condition with constant concentration of component  $B$  described in Section 2.4.3 is used. It is noted that on every corner line and at every corner point of the walls, one cannot determine unknown distribution functions for component  $B$  by using the boundary condition for the same reason as in the duct flow problem. Therefore, the same procedure as in the previous problem is conducted in this problem. Figure 2.6 shows the calculated concentration profile with  $\Delta x = 0.1$  and  $\tau_B = 0.85$ . The solid line and closed circles indicate the analytical solution and the calculated results, respectively. It is seen that the results agree well with the analytical solution. Next, the errors of the calculated results from the analytical solution with various  $\Delta x$  and  $\tau_B$  are examined. It is seen from Equations (2.5.3) and (2.5.5) that  $\Pi_B$  is not directly related to  $D_{BA}$  as long as  $v_{A0}/D_{BA}$  is kept at a constant value. Hence,  $\Pi_B$  is independent of  $\tau_B$  since the effect of  $\tau_B$  appears in macroscopic variables only through  $D_{BA}$ . Thus,  $k$  is in proportion to  $\Delta x$  alone. It follows from the asymptotic theory that the errors are proportional to  $(\Delta x)^2$ . Table 2.2 represents the error norms  $Er_1 = \sum_{x_2} |\Pi_B - \Pi_B^*| / \sum_{x_2} |\Pi_B^*|$  and  $Er_2 = \sqrt{\sum_{x_2} (\Pi_B - \Pi_B^*)^2} / \sqrt{\sum_{x_2} (\Pi_B^*)^2}$  where the sums

are taken over the same 11 nodes between the walls for all cases. It is clearly found that the errors decrease in proportion to  $(\Delta x)^2$  regardless of  $\tau_B$ .

## 2.6 Concluding Remarks

In this Chapter basic theories for the lattice Boltzmann method (LBM) are described and numerical calculations are carried out to demonstrate the validity of the theories. The results are summarized as follows:

1. The asymptotic theory proposed by Sone is applied to the LBM with the fifteen-velocity model and the continuity equation and the Navier-Stokes equations for incompressible fluid are derived. From the fluid-dynamic type equations of the LBM it is found that by using the LBM one can obtain the macroscopic flow velocities and the pressure gradient for incompressible fluid with relative errors of  $O(k^2)$  where  $k$  is a modified Knudsen number which is of the same order as the lattice spacing and is related to a dimensionless relaxation time.
2. A new approach for applying a no-slip boundary condition at a wall is proposed. In the present method unknown distribution functions at the wall are assumed to be an equilibrium distribution function with a counter slip velocity which is determined so that fluid velocity at the wall is equal to the wall velocity. A three-dimensional flow through a square duct with a constant pressure gradient is calculated with the present boundary condition and the accuracy of the method is investigated. From the results it is found that the present boundary condition is accurate to model a no-slip boundary in the LBM.
3. The LBM for a binary fluid mixture with a simple kinetic model is proposed. The asymptotic theory is applied to the LBM for a binary fluid mixture and

fluid-dynamic type equations are obtained. From the fluid-dynamic type equations it is found that by using the LBM for a binary fluid mixture one can obtain the macroscopic concentration of diffusing component with relative errors of  $O(k^2)$ .

## Chapter 3

# Flow Analysis in Porous Structure by LBM

### 3.1 Introduction

In this Chapter, flows in a three-dimensional porous structure are numerically studied. As stated in Section 1.3, the previous studies are mainly based on the volume-averaged approaches to obtain macroscopic properties of flows in porous media. However, in the case of complex porous structures such as with non-uniform porosity, it is important to investigate flow characteristics in porous media from the microscopic point of view. Recently, several studies on the investigation of microscopic behavior occurring at a pore scale have been carried out for relatively low Reynolds numbers. As the Reynolds number increases, on the other hand, it is considered that flow fields in porous media become completely different from those at low Reynolds numbers due to the appearance of unsteady vortices. Thus, it is interesting to study flow characteristics in porous media at high Reynolds numbers, particularly in the transition region from laminar to turbulent flow.

In the present study, the LBM with the fifteen-velocity model is developed and applied to simulations of flows in a three-dimensional porous structure. Flow characteristics at a pore scale and pressure drops through the structure are investigated

at high Reynolds numbers as well as low Reynolds numbers. In addition, flow characteristics in the transition region from laminar to turbulent flow are examined.

## 3.2 Problem

The problem of flow in a three-dimensional porous structure, shown in Figure 3.1, is considered. There exist nine identical spherical bodies in the rectangular domain of  $L_y = L_z = 0.945L_x$ . The body is made up of a lattice block. The equivalent diameter  $D_p$  of the body is  $0.403L_x$ , which is determined by the procedure explained later in Section 3.4. Then the porosity  $\varepsilon$  of the structure is 0.654. The centers of the bodies are located at  $(x/L_x, y/L_y, z/L_z) = (0.21, 0.29, 0.22), (0.21, 0.74, 0.81), (0.22, 0.71, 0.22), (0.23, 0.32, 0.80), (0.48, 0.49, 0.49), (0.75, 0.80, 0.29), (0.78, 0.23, 0.70), (0.78, 0.78, 0.70),$  and  $(0.80, 0.23, 0.29)$ .

## 3.3 Boundary Conditions

Boundary conditions in the LBM, needed for the following simulations, are presented. A no-slip boundary condition is used on the body. A periodic boundary condition with a pressure difference is used at the inlet and outlet. The other faces are considered slip walls.

### No-Slip Boundary Condition on Body

First, the boundary condition on the body is considered. As shown in Figure 3.2 the lattice node  $P$  is a boundary point on the body and  $S$  is a tangent plane on the node  $P$ . Here, let  $\mathbf{n}$  be the normal vector along the line connecting the node  $P$  with the center of the body, and  $\mathbf{t}$  and  $\mathbf{b}$  the unit vectors perpendicular to  $\mathbf{n}$ . The velocity vectors of the particles  $\mathbf{c}_i$  are written in terms of the orthonormal bases as

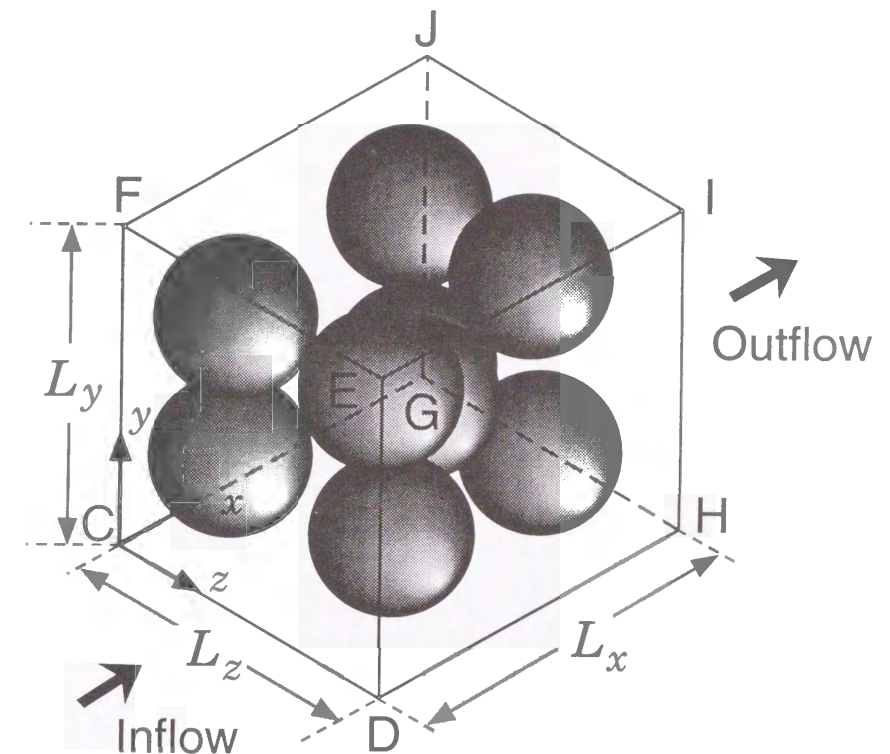


Figure 3.1: Three-dimensional porous structure.

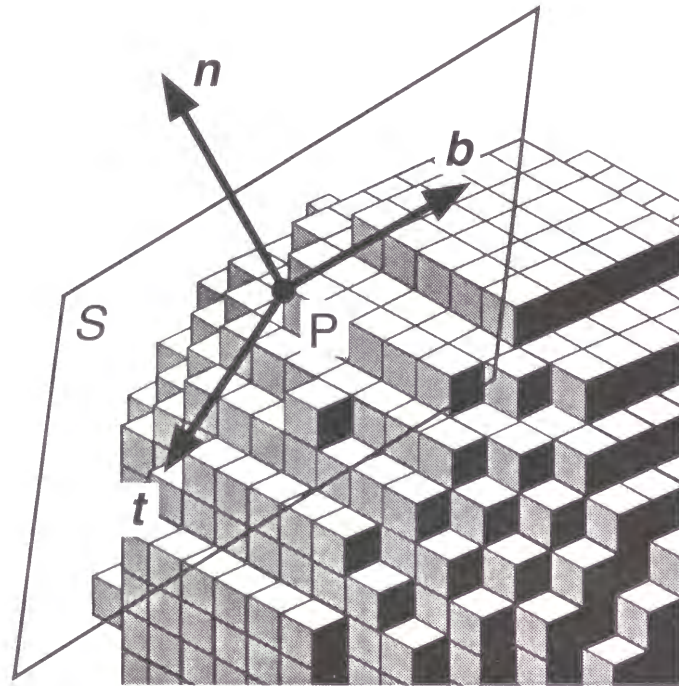


Figure 3.2: Tangent plane  $S$  on the lattice node of body and orthonormal bases  $\mathbf{n}$ ,  $\mathbf{t}$ , and  $\mathbf{b}$ .

$$\mathbf{c}_i = c_{in}\mathbf{n} + c_{it}\mathbf{t} + c_{ib}\mathbf{b}. \quad (3.3.1)$$

As seen from Figure 3.2, at the boundary node P the distribution functions with  $c_{in} > 0$  are unknown. The idea of the present method is the same as that of the no-slip boundary condition at the wall described in Section 2.3.1. The unknown distribution functions are assumed to be the equilibrium distribution functions given by Equation (2.2.12) with two components of a counter slip velocity,  $u'_t$  and  $u'_b$ , as follows:

$$f_i = E_i \rho' \left[ 1 + 3(c_{it}u'_t + c_{ib}u'_b) + \frac{9}{2}(c_{it}u'_t + c_{ib}u'_b)^2 - \frac{3}{2}(u'^2_t + u'^2_b) \right] \quad \text{for } c_{in} > 0, \quad (3.3.2)$$

where  $\rho'$ ,  $u'_t$ , and  $u'_b$  are unknown parameters. The three unknown parameters are determined on the condition that the fluid velocity on the boundary node is equal to zero. Moreover, the fluid density  $\rho_w$  at the boundary node is an unknown quantity and is calculated by Equation (2.2.7). Hence, four equations for the four unknowns are obtained. Assuming that  $u'^2_t$  and  $u'^2_b$  are negligibly small, the solutions are obtained as follows:

$$u'_t = \frac{G}{F}, \quad (3.3.3)$$

$$u'_b = \frac{H}{F}, \quad (3.3.4)$$

$$\rho' = - \frac{\sum_{i(c_{in} \leq 0)} c_{in} f_i}{\sum_{i(c_{in} > 0)} E_i c_{in} (1 + 3c_{it}u'_t + 3c_{ib}u'_b)}, \quad (3.3.5)$$

$$\rho_w = \sum_{i(c_{in} > 0)} E_i \rho' (1 + 3c_{it}u'_t + 3c_{ib}u'_b) + \sum_{i(c_{in} \leq 0)} f_i, \quad (3.3.6)$$

where

$$D_1 = \sum_{i(c_{in} < 0)} c_{it} f_i. \quad (3.3.7)$$

$$D_2 = \sum_{i(c_{in} \leq 0)} c_{in} f_i. \quad (3.3.8)$$

$$D_3 = \sum_{i(c_{in} \leq 0)} c_{ib} f_i. \quad (3.3.9)$$

$$\begin{aligned} F = & 9 \sum_{i(c_{in} > 0)} E_i c_{it} (D_2 c_{it} - D_1 c_{in}) \times \sum_{i(c_{in} > 0)} E_i c_{ib} (D_2 c_{ib} - D_3 c_{in}) \\ & - 9 \sum_{i(c_{in} > 0)} E_i c_{ib} (D_2 c_{it} - D_1 c_{in}) \times \sum_{i(c_{in} > 0)} E_i c_{it} (D_2 c_{ib} - D_3 c_{in}). \end{aligned} \quad (3.3.10)$$

$$\begin{aligned} G = & 3 \sum_{i(c_{in} > 0)} E_i (D_1 c_{in} - D_2 c_{it}) \times \sum_{i(c_{in} > 0)} E_i c_{ib} (D_2 c_{ib} - D_3 c_{in}) \\ & - 3 \sum_{i(c_{in} > 0)} E_i (D_3 c_{in} - D_2 c_{ib}) \times \sum_{i(c_{in} > 0)} E_i c_{it} (D_2 c_{it} - D_1 c_{in}). \end{aligned} \quad (3.3.11)$$

$$\begin{aligned} H = & 3 \sum_{i(c_{in} > 0)} E_i (D_3 c_{in} - D_2 c_{ib}) \times \sum_{i(c_{in} > 0)} E_i c_{it} (D_2 c_{it} - D_1 c_{in}) \\ & - 3 \sum_{i(c_{in} > 0)} E_i (D_1 c_{in} - D_2 c_{it}) \times \sum_{i(c_{in} > 0)} E_i c_{ib} (D_2 c_{ib} - D_3 c_{in}). \end{aligned} \quad (3.3.12)$$

Substituting Equations (3.3.3)-(3.3.5) into Equation (3.3.2) all the unknown distribution functions on the boundary node are determined.

However, it should be noted that the counter slip velocity often causes numerical instabilities at high Reynolds numbers. One reason for the fact would be that the matrix representing the system of the linear algebraic Equations (3.3.3)–(3.3.6) becomes ill-conditioned (nearly singular). Thus, Equation (3.3.10), which is denominator in Equations (3.3.3) and (3.3.4), approaches zero as the Reynolds number increases. In preliminary computations of the three-dimensional duct flow problem

described in Section 2.5.1, the magnitude of the counter slip velocity decreases as  $\tau$  and  $\Delta x$  become smaller. In the following simulations, since  $\Delta x$  is kept at about  $1/70$  and  $\tau$  is changed in the range of small values (approximately between 0.52 and 0.55) at high Reynolds numbers, it is estimated by the extrapolation that the value of the counter slip velocity is at most about  $3 \sim 4\%$  of the main flow velocity. Therefore, two components of the counter slip velocity,  $u'_t$  and  $u'_b$ , are set to be zero. Then we have only one unknown parameter  $\rho'$ , which is reduced to

$$\rho' = - \frac{\sum_{i(c_{in} < 0)} c_{in} f_i}{\sum_{i(c_{in} > 0)} E_i c_{in}}. \quad (3.3.13)$$

### Periodic Boundary Condition at Inlet and Outlet

A periodic boundary condition with a pressure difference  $\Delta p$  is used at the inlet and outlet described in Section 2.3.2.

On the corner line, e.g., on the line CD in Figure 3.1,  $f_2$ ,  $f_8$ ,  $f_{10}$ ,  $f_{11}$ ,  $f_{13}$ ,  $f_3$ ,  $f_9$ , and  $f_{14}$  are unknown. In these unknown distribution functions,  $f_2$ ,  $f_8$ ,  $f_{10}$ ,  $f_{11}$ , and  $f_{13}$  are determined by the boundary condition at the inlet, and the others,  $f_3$ ,  $f_9$ , and  $f_{14}$ , are determined by the slip boundary condition described below.

### Slip Wall Boundary Condition

Finally, a slip boundary conditions at the side wall is presented. For example, at the lattice node on the face CDHG in Figure 3.1,  $f_3$ ,  $f_8$ ,  $f_9$ ,  $f_{11}$ , and  $f_{14}$  are unknown distribution functions and simply determined as follows:

$$\left. \begin{aligned} f_3 &= f_6, \\ f_8 &= f_{10}, \\ f_9 &= f_{15}, \\ f_{11} &= f_{13}, \\ f_{14} &= f_{12}, \end{aligned} \right\} \quad (3.3.14)$$

On the corner line, e.g., on the line DH,  $f_3$ ,  $f_8$ ,  $f_9$ ,  $f_{11}$ ,  $f_{14}$ ,  $f_7$ ,  $f_{12}$ , and  $f_{13}$  are unknown. In these unknowns,  $f_3$ ,  $f_8$ ,  $f_9$ ,  $f_{11}$ , and  $f_{14}$  are determined by Equation (3.3.14), and the others,  $f_7$ ,  $f_{12}$ , and  $f_{13}$ , are determined by regarding the line DH as a part of the face EDHI, i.e.,

$$\left. \begin{aligned} f_7 &= f_4, \\ f_{12} &= f_{15}, \\ f_{13} &= f_{10}, \end{aligned} \right\} \quad (3.3.15)$$

Moreover, the unknown distribution functions at the vertex can be determined by the combination of the above-mentioned conditions. For example, at the vertex D, the unknown distribution functions are  $f_2$ ,  $f_3$ ,  $f_7$ ,  $f_8$ ,  $f_9$ ,  $f_{10}$ ,  $f_{11}$ ,  $f_{12}$ ,  $f_{13}$ , and  $f_{14}$ . In these unknown distribution functions,  $f_2$ ,  $f_8$ ,  $f_{10}$ ,  $f_{11}$ , and  $f_{13}$ , are determined by the procedure at the inlet and the others,  $f_3$ ,  $f_7$ ,  $f_9$ ,  $f_{12}$ , and  $f_{14}$ , are determined by the above-mentioned slip boundary condition on the side.

### 3.4 Computational Conditions

The whole domain is divided into  $73 \times 69 \times 69$  cubic lattice in the  $x$ -,  $y$ -, and  $z$ -directions. The diameter of the circumscribed sphere of the body is  $28.4\Delta x$ . It is expected that the equivalent diameter of the body,  $D_p$ , is larger than that of the circumscribed sphere, but one cannot determine the value of  $D_p$  in advance of

calculations. In this study, we tried to determine the value of  $D_p$  by comparing a calculated pressure drop with the Blake-Kozeny equation at the lowest Reynolds number as explained below. The determined value of  $D_p$  is equal to  $29.4\Delta x$ , and the porosity  $\varepsilon$  of the structure is 0.654. In the calculations, the pressure difference  $\Delta p$  between the inlet and outlet and the fluid viscosity  $\mu$  are changed so that the range of the Reynolds number,  $\text{Re} = \bar{\rho}_{\text{in}} \bar{u}_{\text{in}} D_p / \mu$ , is  $0.842 \leq \text{Re} \leq 164$ , where  $\rho_{\text{in}} (= 1)$  and  $\bar{u}_{\text{in}}$  are the time- and space-averaged density and velocity at the inlet after transitional flows, respectively. The initial conditions for the flow velocity and density are  $\mathbf{u} = 0$  and  $\rho = 1$  in the whole domain. In preliminary computations,  $38 \times 35 \times 35$  and  $49 \times 46 \times 46$  cubic lattices were also used. Then almost grid-independent results were obtained at low Reynolds numbers, but numerical instabilities occurred at high Reynolds numbers when the coarse grids were used.

## 3.5 Results and Discussion

### 3.5.1 Flow Characteristics and Pressure Drops

Figures 3.3–3.5 show the calculated results of velocity vectors on the different planes ( $y/L_y = 0.17$ , 0.62, and  $x/L_x = 0.51$ ) for various Reynolds numbers after transitional flows. In these figures, the length of vectors is normalized so that the  $\bar{u}_{\text{in}}$  has the same length in spite of different Reynolds numbers, and the bodies in the structure are depicted by the spheres with the equivalent diameter  $D_p$ . It is found from Figures 3.3–3.5 that at low Reynolds number  $\text{Re} = 0.842$ , the fluid flow avoids the bodies and goes through open spaces. At  $\text{Re} = 29.3$ , on the other hand, the flow separations begin to occur and weak vortices appear behind the bodies. At  $\text{Re} = 164$ , the vortices behind the bodies grow three-dimensionally and hence the flow field on  $x/L_x = 0.51$  is completely different from those at the lower Reynolds

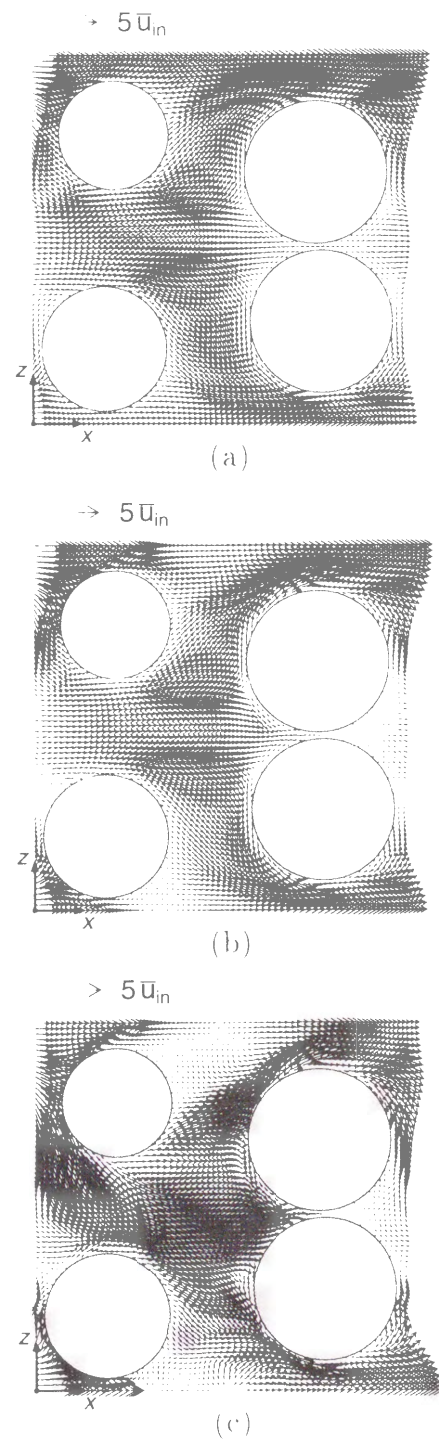


Figure 3.3: Velocity vectors on the plane  $y/L_y = 0.17$  in the porous structure for various Reynolds numbers: (a)  $Re = 0.842$ ,  $\bar{u}_{in} = 4.29 \times 10^{-3}$ ; (b)  $Re = 29.3$ ,  $\bar{u}_{in} = 1.86 \times 10^{-2}$ ; (c)  $Re = 164$ ,  $\bar{u}_{in} = 4.46 \times 10^{-2}$ .

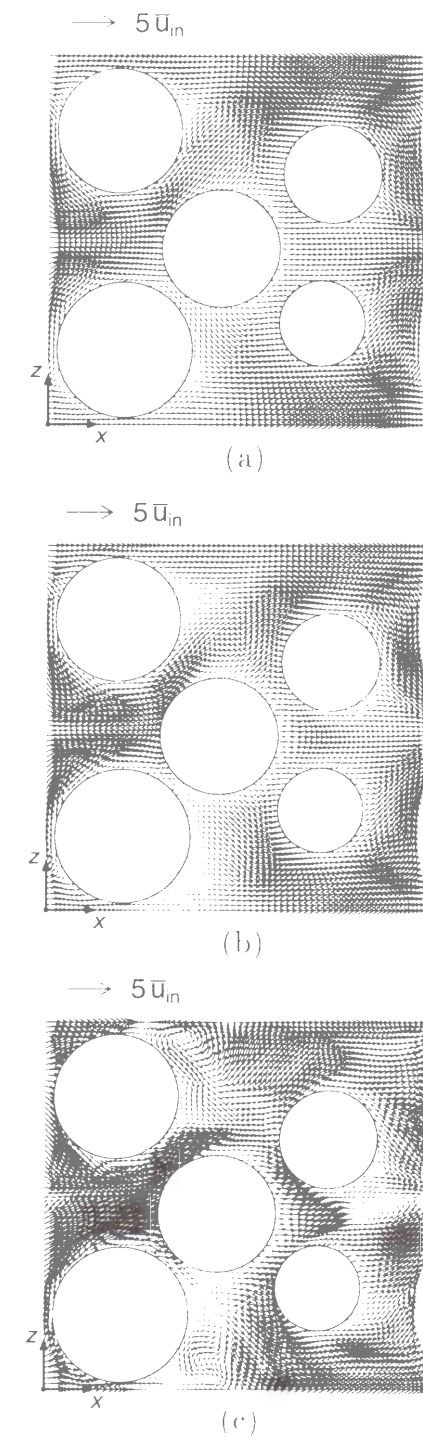


Figure 3.4: Velocity vectors on the plane  $y/L_y = 0.62$  in the porous structure for various Reynolds numbers: (a)  $Re = 0.842$ ,  $\bar{u}_{in} = 4.29 \times 10^{-3}$ ; (b)  $Re = 29.3$ ,  $\bar{u}_{in} = 1.86 \times 10^{-2}$ ; (c)  $Re = 164$ ,  $\bar{u}_{in} = 4.46 \times 10^{-2}$ .

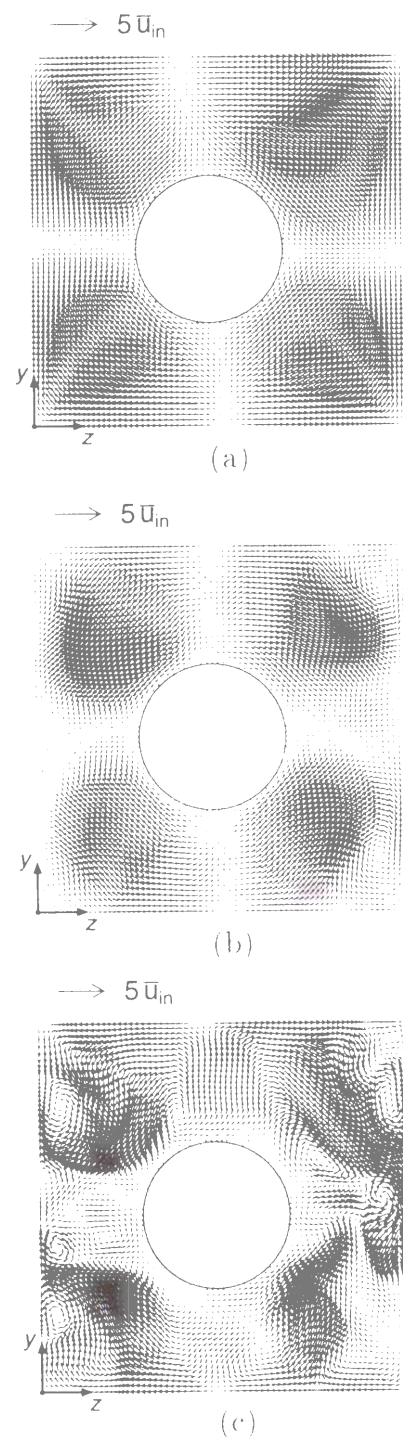


Figure 3.5: Velocity vectors on the plane  $x/L_x = 0.51$  in the porous structure for various Reynolds numbers: (a)  $Re = 0.842$ ,  $\bar{u}_{in} = 4.29 \times 10^{-3}$ ; (b)  $Re = 29.3$ ,  $\bar{u}_{in} = 1.86 \times 10^{-2}$ ; (c)  $Re = 164$ ,  $\bar{u}_{in} = 4.46 \times 10^{-2}$ .

numbers. Also, it is found that at the high Reynolds numbers the strength of each vortex varies as time goes on, and the flow field becomes time-dependent. It is noted that the time variation of the space-averaged velocity at the inlet in this case is only about 2% of the mean value in spite of the large time variations of the local velocity fields as shown later (e.g. Figures 3.8, 3.10, and 3.12).

Finally, the calculated results of pressure drops are compared with well-known empirical equations based on experimental data. Figure 3.6 shows the dimensionless pressure drops  $(\Delta p / (\bar{\rho}_{in} \bar{u}_{in}^2)) \cdot (D_p / L_x) \cdot (\varepsilon^3 / (1 - \varepsilon))$  versus the modified Reynolds numbers  $Re' = Re / (1 - \varepsilon)$ . It is noted that the porosity  $\varepsilon$  of the structure depends only on  $D_p$  as long as the whole rectangular domain is unchanged. As mentioned above, we tried to determine the value of  $D_p$  by comparing the calculated pressure drop with the Blake-Kozeny equation at the lowest Reynolds number. The error bar at the lowest Reynolds number in Figure 3.6 shows the range of the results calculated by changing the value of  $D_p$  between  $28.4\Delta x$  and  $30.4\Delta x$ . Comparing the calculated results with the Blake-Kozeny equation, it was found that a good agreement is obtained with  $D_p = 29.4\Delta x$ , as shown by the closed circle in Figure 3.6. Then the same value of  $D_p$  was used for other Reynolds numbers. It is seen from Figure 3.6 that the calculated results of the pressure drops agree well with the empirical equations for the wide range of the Reynolds numbers, although at the high Reynolds numbers the calculated results become a little smaller than the Ergun equation. It is also found from Figures 3.3–3.6 that the region of the Reynolds numbers where the pressure drops deviate from the Blake-Kozeny equation corresponds to the appearance of the vortices behind the bodies in the structure.

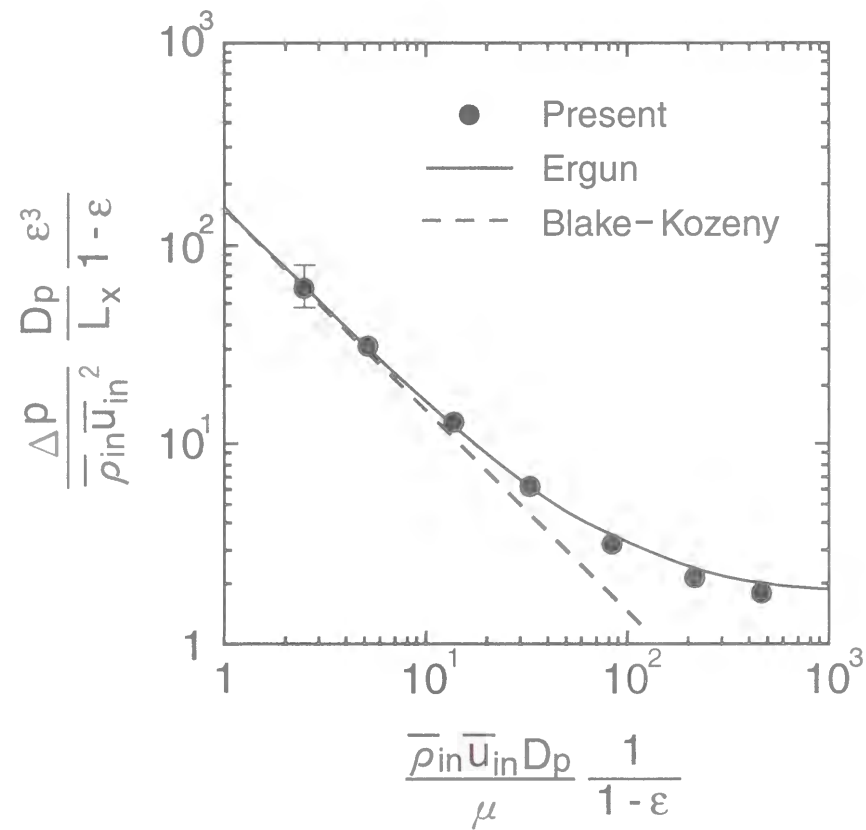


Figure 3.6: Pressure drops versus Reynolds numbers in the porous structure: •, the present calculated results; - - -, the Blake-Kozeny equation; —, the Ergun equation. The error bar indicates the range of calculated results by changing  $D_p$  between  $28.4\Delta x$  and  $30.4\Delta x$ .

### 3.5.2 Analysis of Unsteady Flows

Next, in order to investigate the characteristics of the transition from laminar to turbulent flow, the velocity fluctuations, the power spectra, and the turbulence intensities are calculated at three different points in the structure. These points are located at  $(x/L_x, y/L_y, z/L_z) = (0.45, 0.62, 0.09)$ ,  $(0.51, 0.84, 0.14)$ , and  $(0.55, 0.17, 0.88)$ . In the following these points are referred to as  $P_1, P_2$ , and  $P_3$ , respectively. These points are depicted by the symbol  $\boxtimes$  in Figure 3.7. The point  $P_1$  is located in the wake behind a body. The point  $P_2$  is, on the other hand, located in front of a body and the fluid is affected by approaching flows. Also, the magnitude of the time-averaged flow velocity at the point  $P_2$  is largest in the three points. Finally, the point  $P_3$  is located in front of a body and behind another body. Thus, the fluid at the point  $P_3$  is affected by both flow characteristics.

#### Fluctuations and Power Spectra

Figure 3.8 shows the fluctuations of the  $x$ -component of the flow velocity,  $u_x$ , in the range of  $84.9 \leq Re \leq 164$  at the point  $P_1$ . In the following analysis, the calculated results of flow velocity after transitional states are used. First, at  $Re = 84.9$  flow velocity is time-independent, but at  $Re = 94.3$  a periodic sinusoidal fluctuation with almost constant amplitude and frequency can be seen. Then at  $Re = 107$ , the sinusoidal fluctuation is maintained, although the amplitude of the fluctuation becomes a little larger. At  $Re = 127$ , on the other hand, it is expected that the velocity fluctuation has different frequency components because the amplitude and frequency slightly change with time. However, it should be noted that one cannot determine only from the results of the velocity fluctuations whether the frequency components are incommensurate or harmonic with each other. Moreover, at  $Re = 145$  and  $164$ ,

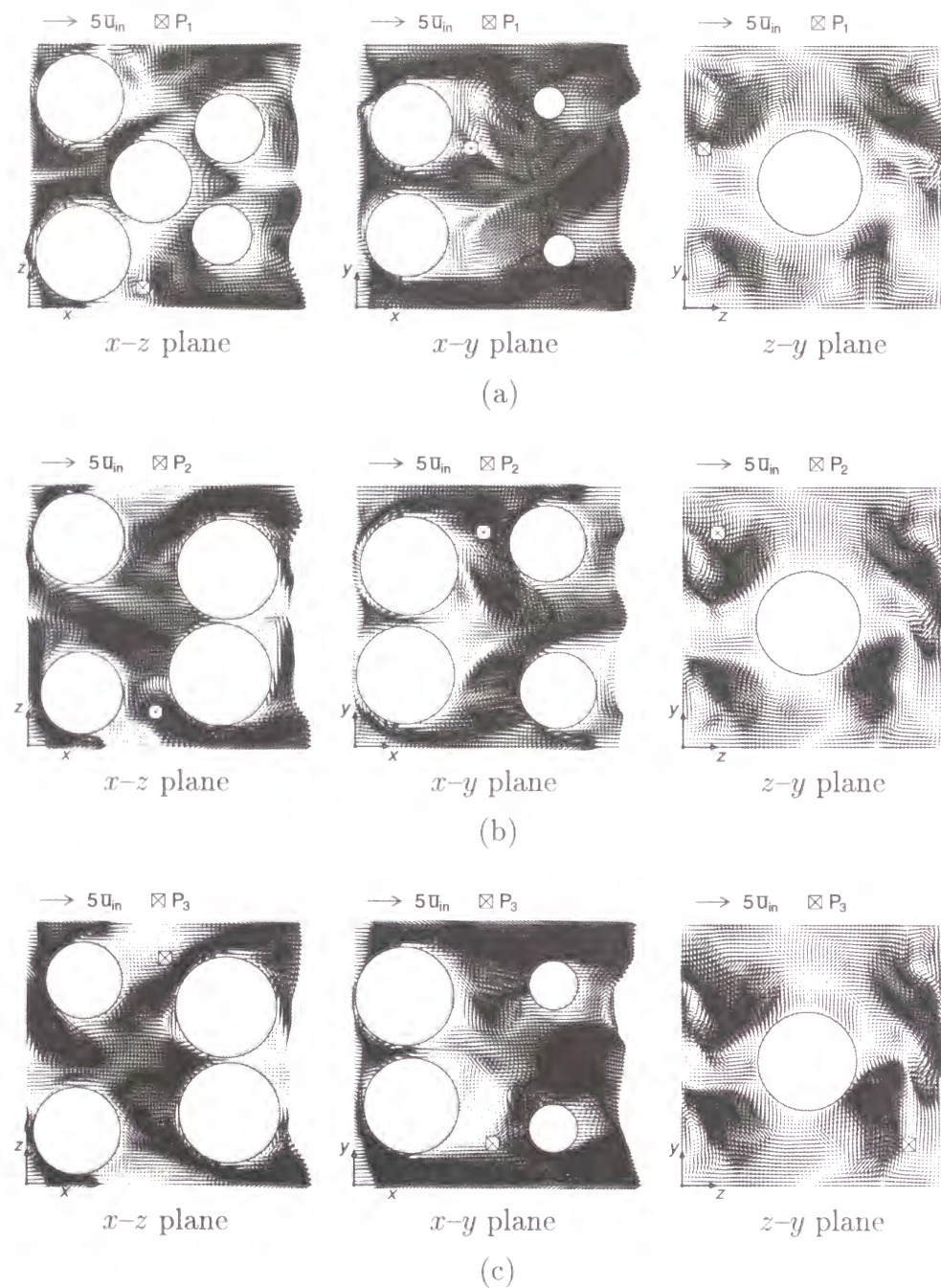


Figure 3.7: Velocity vectors at  $Re = 127$  and the location of the points,  $P_1$ ,  $P_2$ , and  $P_3$  (indicated by  $\boxtimes$ ), where the fluctuations of the flow velocity are investigated: (a)  $P_1$ ,  $(x/L_x, y/L_y, z/L_z) = (0.45, 0.62, 0.09)$ ; (b)  $P_2$ ,  $(x/L_x, y/L_y, z/L_z) = (0.51, 0.84, 0.14)$ ; (c)  $P_3$ ,  $(x/L_x, y/L_y, z/L_z) = (0.55, 0.17, 0.88)$ .

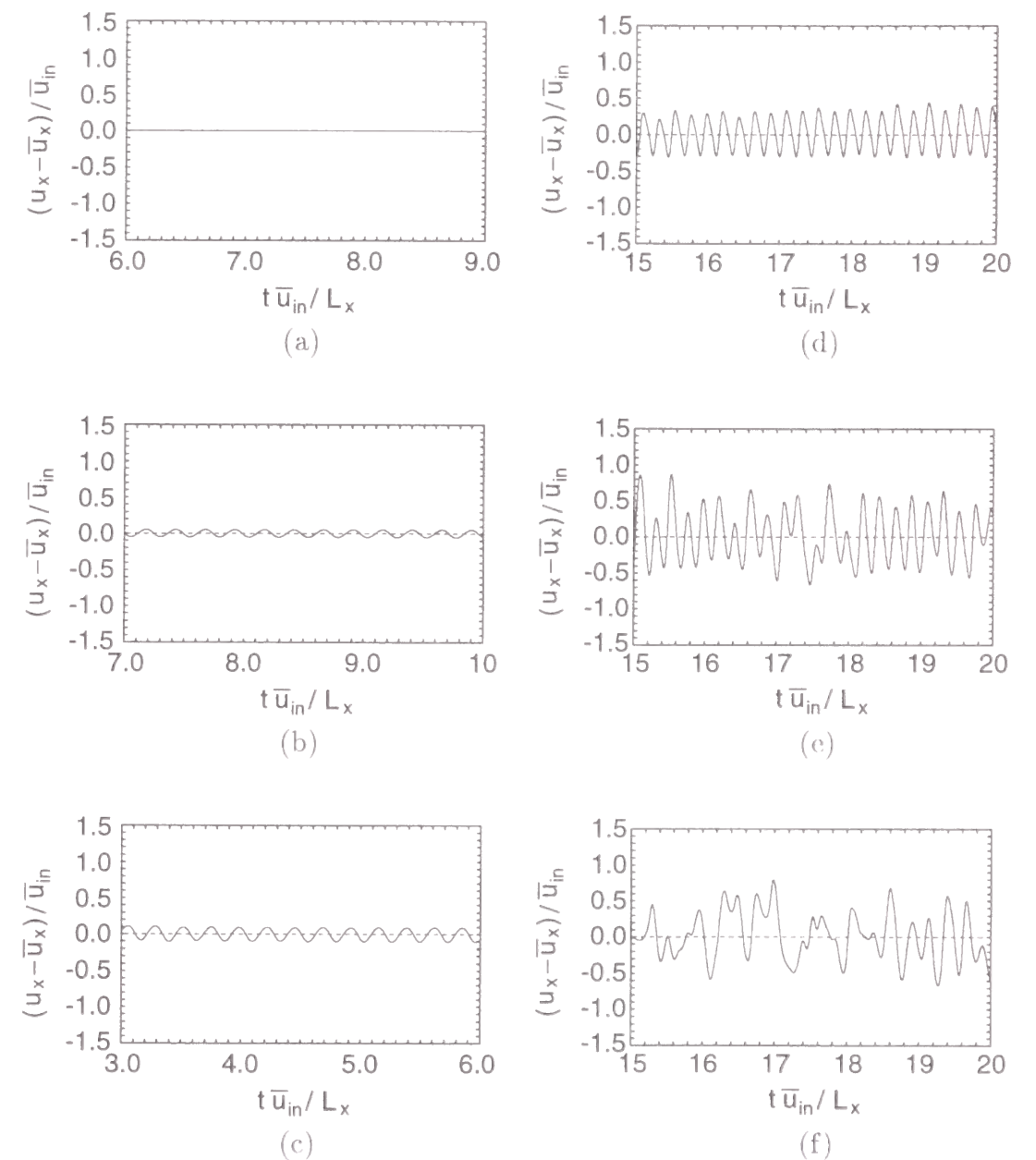


Figure 3.8: Fluctuation of the x-component of the flow velocity at the point  $P_1$ .  $\bar{u}_x$  is the time-averaged value of  $u_x$ : (a)  $Re = 84.9$ ; (b)  $Re = 94.3$ ; (c)  $Re = 107$ ; (d)  $Re = 127$ ; (e)  $Re = 145$ ; (f)  $Re = 164$ .

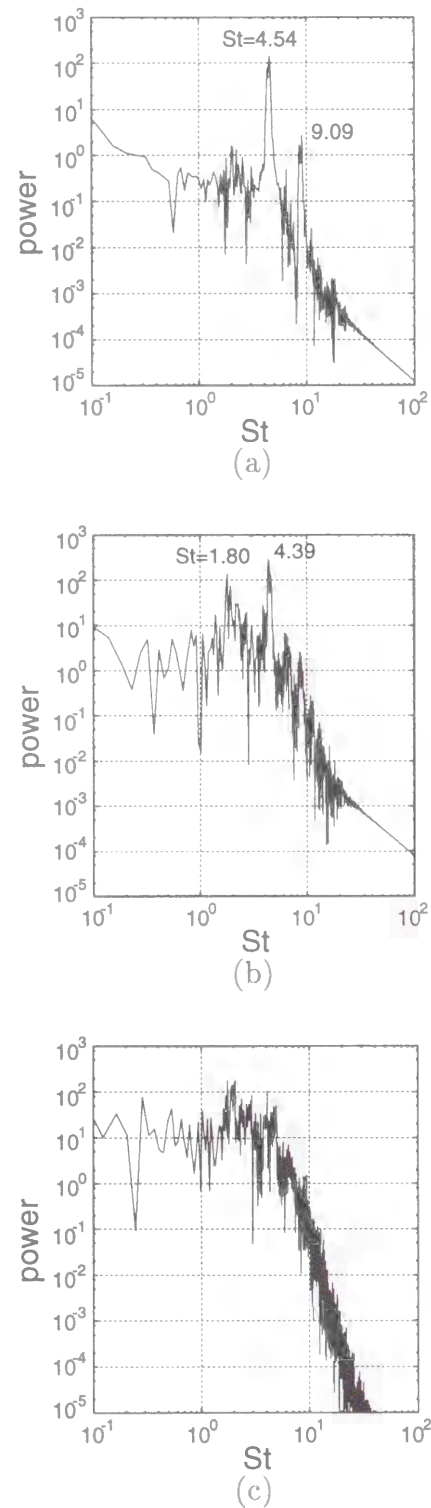


Figure 3.9: Power spectra of the velocity fluctuation at the point  $P_1$ .  $St$  is the Strouhal number  $St = FL_x/\bar{u}_{in}$ , where  $F$  is a frequency: (a)  $Re=127$ ; (b)  $Re=145$ ; (c)  $Re=164$ .

the amplitude becomes still larger and their magnitude changes with time in an irregular manner. Next, the power spectra of the velocity fluctuation are calculated. Here, only the typical results at  $Re = 127, 145$ , and  $164$  are shown in Figure 3.9. In the analysis, the number of sampling data is 40,000 during dimensionless time  $t\bar{u}_{in}/L_x = 18.9, 21.6$ , and  $24.4$  at  $Re = 127, 145$ , and  $164$ , respectively. In Figure 3.9 the horizontal axis represents the Strouhal number  $St = FL_x/\bar{u}_{in}$ , where  $F$  is a frequency. At  $Re = 127$ , it is seen that the power spectrum has distinct peaks at  $St = 4.54$  and its harmonic,  $St = 9.09$ . Thus, the behavior of the velocity fluctuation in Figure 3.8(d) is considered periodic with a single fundamental frequency. At  $Re = 145$ , on the other hand, two peaks appear at  $St = 1.80$  and  $4.39$ , which are both different from above-mentioned frequencies at  $Re = 127$ . It is considered that these two frequencies are expected to be incommensurate, that is, the ratio of these two frequencies is irrational. This means that the behavior of the fluctuation is quasi-periodic, or double-periodic with the two different fundamental frequencies. However, it is noted that one cannot decide whether this is true only from the results of the power spectrum. Besides, at  $Re = 164$  since the power spectrum has no distinct peaks, it is considered that a non-periodic fluctuation occurs. Therefore, from these results the following conclusions are obtained. At the point  $P_1$ , the steady laminar flow is at  $Re = 84.9$ . The unsteady laminar flow occurs at  $Re = 94.3$ , and it is still maintained at  $Re = 107$  and  $127$ . Then the transition from laminar to turbulent flow begins to occur at  $Re = 145$ .

Next, the same analyses are carried out at the points  $P_2$  and  $P_3$ . The fluctuations of the  $x$ -component of the flow velocity and their power spectra at the points are shown in Figures 3.10–3.13. At the point  $P_2$  (Figure 3.10), the flow velocity is time-independent at  $Re = 84.9$ . When the Reynolds number becomes  $Re = 94.3$ ,

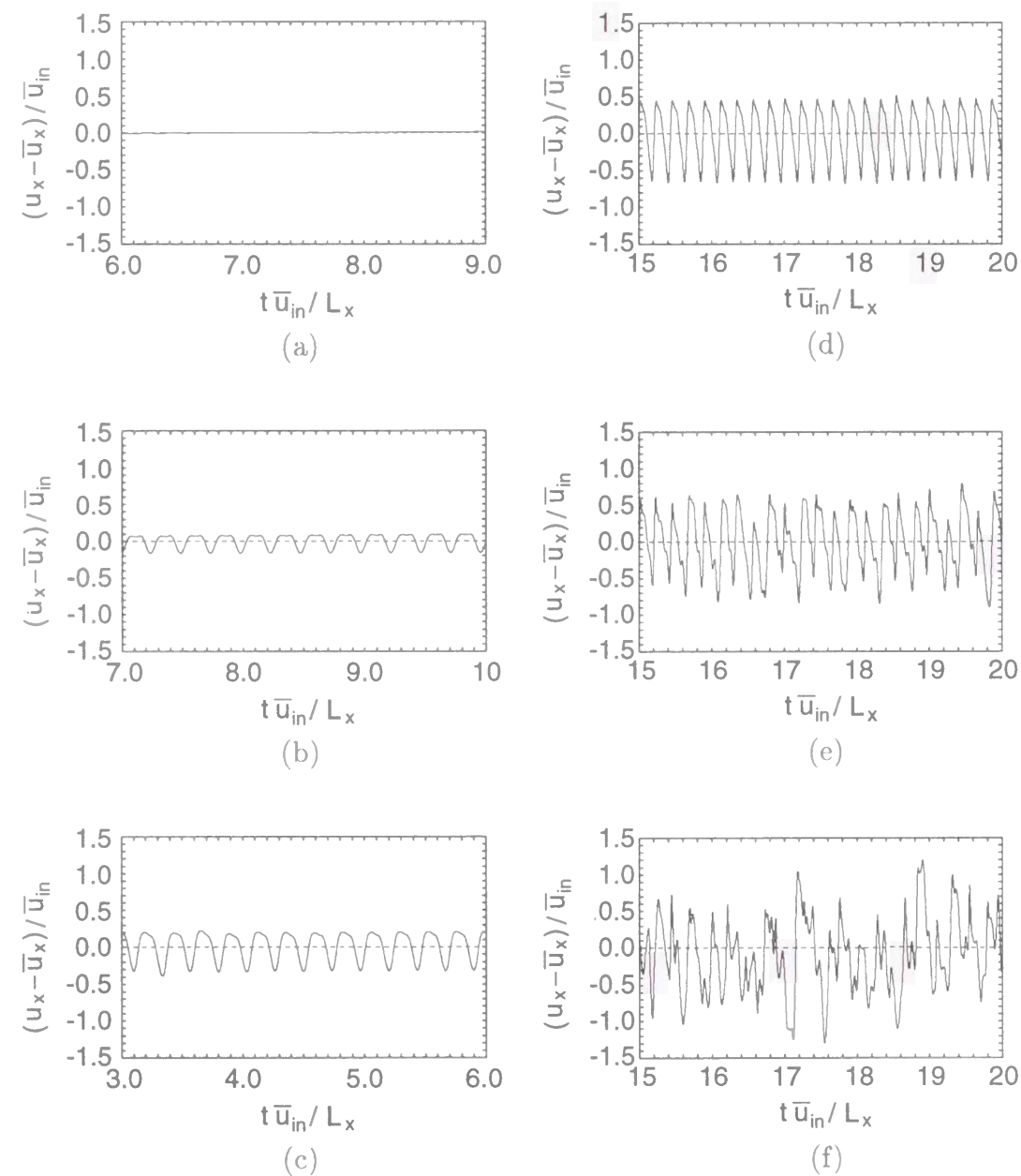


Figure 3.10: Fluctuation of the  $x$ -component of the flow velocity at the point  $P_2$ .  $\bar{u}_x$  is the time-averaged value of  $u_x$ : (a)  $Re = 84.9$ ; (b)  $Re = 94.3$ ; (c)  $Re = 107$ ; (d)  $Re = 127$ ; (e)  $Re = 145$ ; (f)  $Re = 164$ .

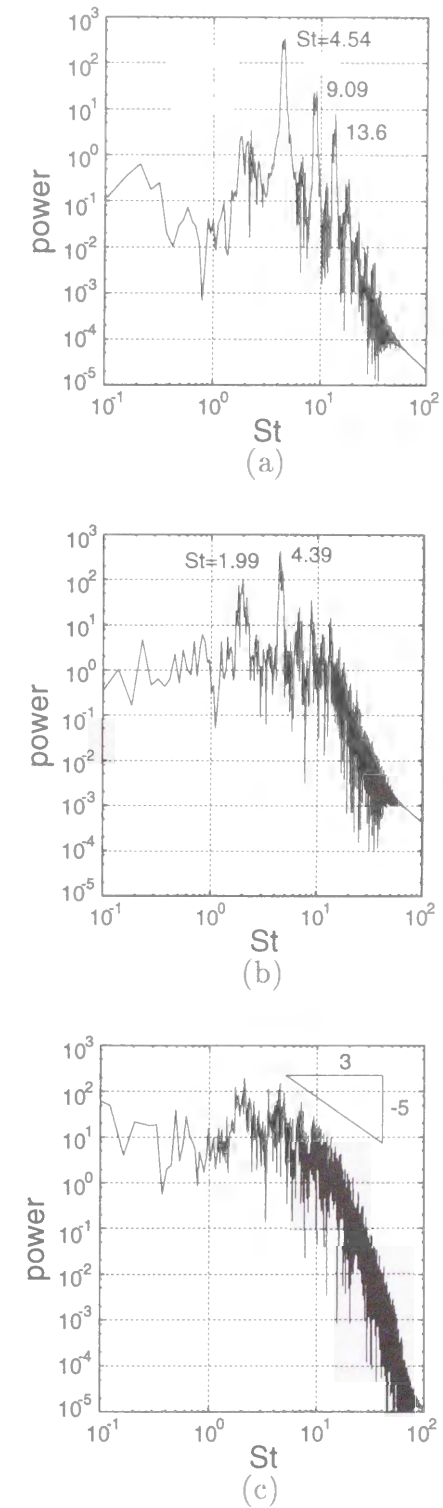


Figure 3.11: Power spectra of the velocity fluctuation at the point  $P_2$ .  $St$  is the Strouhal number  $St = FL_x / \bar{u}_{in}$ , where  $F$  is a frequency: (a)  $Re = 127$ ; (b)  $Re = 145$ ; (c)  $Re = 164$ .

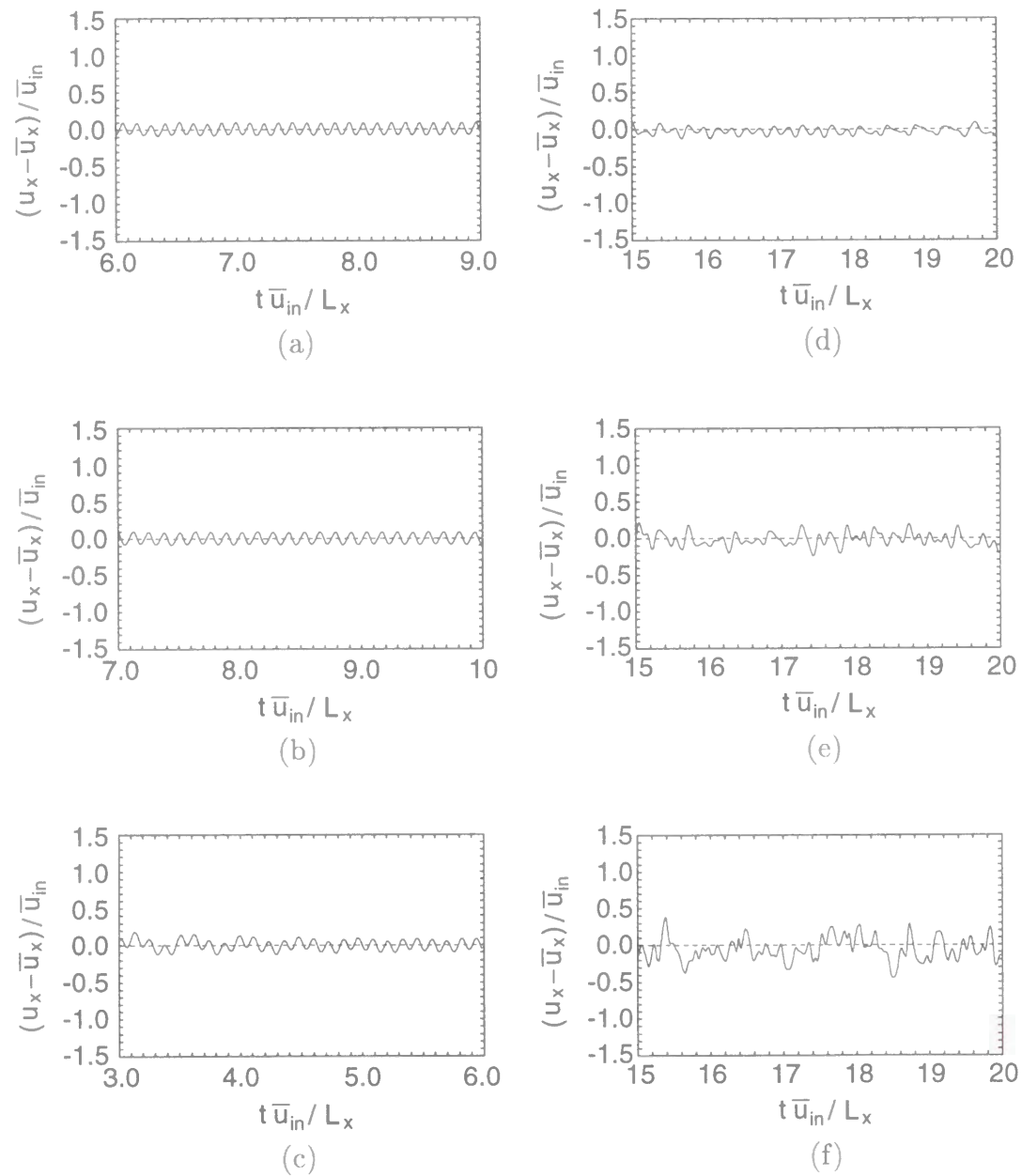


Figure 3.12: Fluctuation of the  $x$ -component of the flow velocity at the point  $P_3$ .  $\bar{u}_x$  is the time-averaged value of  $u_x$ : (a)  $Re = 84.9$ ; (b)  $Re = 94.3$ ; (c)  $Re = 107$ ; (d)  $Re = 127$ ; (e)  $Re = 145$ ; (f)  $Re = 164$ .

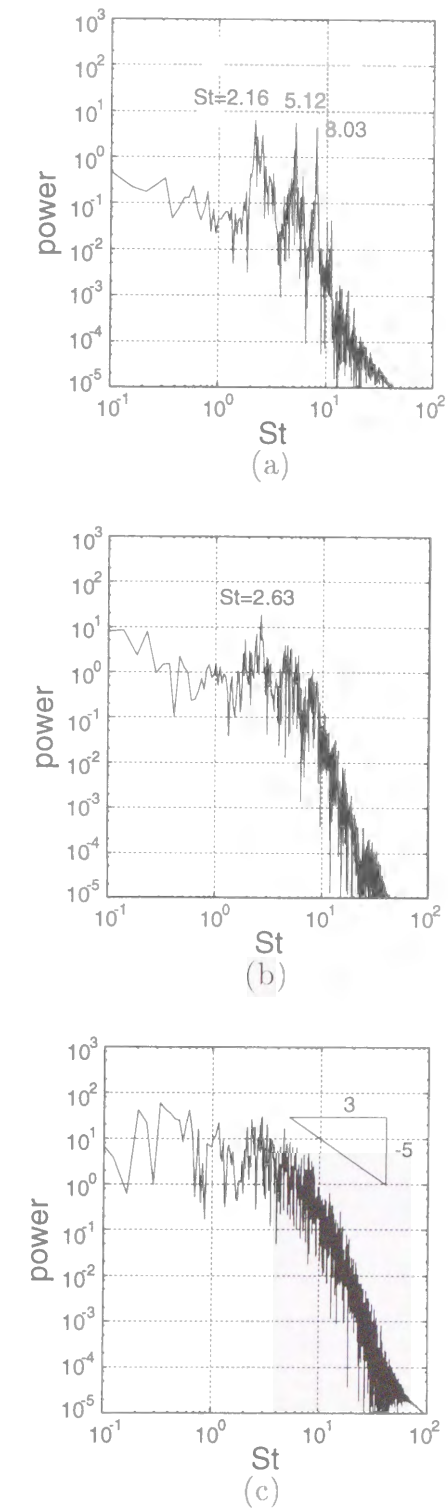


Figure 3.13: Power spectra of the velocity fluctuation at the point  $P_3$ .  $St$  is the Strouhal number  $St = FL_x / \bar{u}_{in}$ , where  $F$  is a frequency: (a)  $Re = 127$ ; (b)  $Re = 145$ ; (c)  $Re = 164$ .

on the other hand, it is found from Figure 3.10(b) that the appearing fluctuation is almost periodic but not sinusoidal. That is, the upper portion of the wave shape is flat and the lower is sharp. In addition, the amplitude of the fluctuation is very large, and especially at  $Re = 145$  and  $164$  the fluctuation has many high-frequency components. Next, from the results of the power spectra (Figure 3.11), it is considered that the transition from laminar to turbulent flow occurs at  $Re = 145$  for the same reason as that at the point  $P_1$ . At  $Re = 164$  broad-band power spectrum appears over a wide range of frequency and the slope of the power spectrum is nearly  $-5/3$  around  $4 \leq St \leq 20$ . In general, the appearance of the slope of  $-5/3$  in the power spectrum is known as a hallmark of turbulence. However, it can be seen that the flow is not completely turbulent because the weak peaks are still remained around  $St = 2$ . Therefore, it is considered that at  $Re = 164$  the flow is just in the early stage of turbulence. Finally, at the point  $P_3$  (Figure 3.12), it should be noted that the periodic fluctuation already occurs at  $Re = 84.9$ , while it does not appear at the points  $P_1$  and  $P_2$ . At  $Re = 68.1$  the flow does not change with time although the result is not shown. As the Reynolds number increases, the fluctuation has small amplitude but more high-frequency components and becomes very complicated. Next, from the results of the power spectra (Figure 3.13), it is found that at  $Re = 127$  the quasi-periodic or triple-periodic fluctuation with three different fundamental frequencies already appears, and thus the transition from laminar to turbulent flow begins to occur. At  $Re = 145$  the fluctuation has almost broad-band power spectrum except for one peak at  $St = 2.63$ , and at  $Re = 164$  completely broad-band power spectrum appears. Therefore, it is found from the above-mentioned results that at the point  $P_3$  the Reynolds numbers where the velocity fluctuation begins and the transition from laminar and turbulent flow occurs

are both lowest in the three points.

### Turbulence Intensity

Finally, turbulence intensity of the  $x$ -component of flow velocity at the three points is calculated in the range of  $68.1 \leq Re \leq 164$ . The turbulence intensity  $I_x$  is defined as

$$I_x = \frac{\sqrt{\overline{(u_x - \bar{u}_x)^2}}}{\bar{u}_{in}}, \quad (3.5.1)$$

where  $\overline{(u_x - \bar{u}_x)^2}$  represents the time-averaged value. In the analysis, the number of sampling data is 8,000 in dimensionless time  $t\bar{u}_{in}/L_x = 2.45, 2.53, 2.81, 3.19, 3.78, 4.05, 4.33, 4.57$ , and  $4.89$  at  $Re = 68.1, 84.9, 94.3, 107, 127, 136, 145, 153$ , and  $164$ , respectively. Figure 3.14 shows the calculated turbulence intensity versus Reynolds numbers. It is found from this figure that at the point  $P_1$  the value of  $I_x$  is approximately zero at  $Re \leq 84.9$ , where the flow velocity does not fluctuate, and increases gradually with increasing  $Re$ . On the contrary, at the point  $P_2$  the value of  $I_x$  increases at  $84.9 \leq Re \leq 145$ , decreases slightly around  $Re \approx 150$ , and then increases again at  $Re \geq 150$ . Also, at the point  $P_3$  the dependence of  $I_x$  on the Reynolds number is quite similar to that at the point  $P_2$ , although the magnitude of the turbulence intensity is much smaller than the previous one. That is,  $I_x$  increases at  $68.1 \leq Re \leq 100$ , decreases slightly at  $100 \leq Re \leq 135$ , and then increases again at  $Re \geq 135$ . From the results in the preceding Section as well as in this Section, the following conclusions are obtained. The value of the turbulence intensity of the flow velocity first increases with increasing  $Re$  in the unsteady laminar flow region and in the early stage of transition from laminar to turbulent flow, then decreases slightly, and finally increases again around a critical Reynolds number, where the flow is considered to

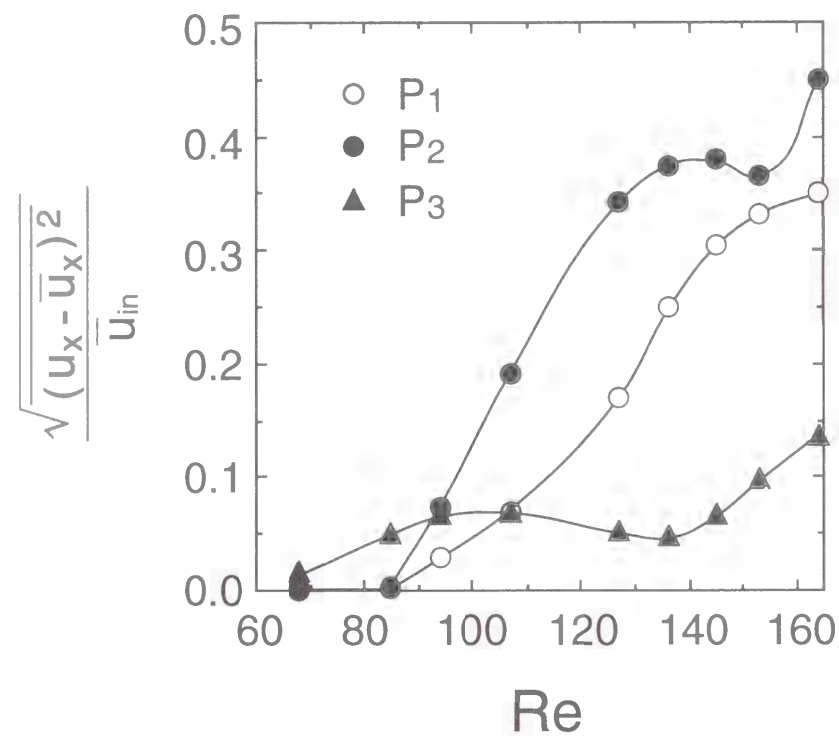


Figure 3.14: Turbulence intensity of the  $x$ -component of flow velocity versus Reynolds numbers.

become turbulent. At the point  $P_1$ , on the other hand, the value of  $I_x$  monotonously increases in the range of  $Re \leq 164$  and the slope of  $-5/3$  in the power spectrum cannot be clearly seen. Therefore, it is considered that the transition from laminar to turbulent does not occur at  $Re = 164$ .

Finally, the same analyses were carried out for the  $y$ - and  $z$ -components of the flow velocity at the three points, though the figures of these results are not shown. At the point  $P_2$ , we can see that there are a little difference in the results at  $Re = 164$ . That is, in the power spectra of the  $y$ - and  $z$ -components of the flow velocity, weak peaks remain around  $St \approx 4.5$  as well as around  $St \approx 2$ . In addition, the turbulence intensity of the  $y$ - and  $z$ -components of the flow velocity at  $Re = 164$  still decreases, while the turbulence intensity of the  $x$ -component begins to increase again. Hence, it is found that the behavior of the transition from laminar to turbulent flow depends on the components of the flow velocity at the point  $P_2$ . At the points  $P_1$  and  $P_3$ , on the other hand, almost the same results are obtained in spite of the components of the flow velocity.

### 3.6 Concluding Remarks

The LBM with the fifteen-velocity model is applied to simulations of fluid flows in a three-dimensional porous structure. Flow fields at a pore scale and pressure drops through the structure are calculated for various Reynolds numbers. Also, the characteristics of unsteady flows in the structure at relatively high Reynolds numbers are investigated. From these results the following conclusions are obtained:

1. The calculated pressure drops agree well with the Blake–Kozeny equation for low Reynolds numbers and with the Ergun equation for high Reynolds numbers.

2. When the Reynolds number, defined by the superficial velocity and the equivalent diameter of the body, is higher than about 80, unsteady vortices appear behind the spherical bodies and the flow fields become time-dependent.
3. From the fluctuation of the flow velocity and its power spectrum, it is found that in the transition region from laminar to turbulent flow a periodic fluctuation appears at first, then the fluctuation becomes quasi-periodic, and finally a non-periodic and complicated fluctuation appears.
4. It is found that the Reynolds numbers where the velocity fluctuation begins and the transition from laminar and turbulent flow occurs depend on the positions in the structure.
5. Turbulence intensity of the flow velocity first increases with increasing Reynolds number in the unsteady laminar flow region and in the early stage of transition from laminar to turbulent flow, then decreases slightly, and finally increases again around a critical Reynolds number, where the flow is considered to become turbulent.

## Chapter 4

# Flow and Mass Transfer Analysis in Porous Structure by LBM

### 4.1 Introduction

In this Chapter, flow and mass transfer in the three-dimensional porous structure are numerically studied. As shown in Chapter 3, the flow characteristics in the porous structure at high Reynolds numbers are very complicated and quite different from those at low Reynolds numbers. In particular, concerning heat/mass transfer in porous media at high Reynolds numbers, the volume-averaged approaches often give the incorrect estimate of macroscopic properties due to the turbulent vortex mixing, which is referred to as ‘dispersion’ (Koch & Brady 1985; Hsu & Cheng 1990) intrinsic to turbulent flows through porous media. Therefore, it is essential to investigate the relation between heat/mass transfer and fluid flow characteristics from the microscopic point of view.

In the present study, the LBM for a binary fluid mixture is developed and applied to the problems of flow and mass transfer in the porous structure. The applicability of the method to calculations of concentration profiles and of Sherwood numbers in the structure is investigated.

## 4.2 Problem

The problem of flow and mass transfer in the three-dimensional porous structure, shown in Figure 3.1, is considered. The details of the structure are explained in Chapter 3.

In this study, it is assumed that the fluid of  $A$ -species flows through the structure and  $B$ -species is diffused from the bodies. A periodic boundary condition with pressure difference is considered at the inlet and outlet. A slip wall boundary condition is applied to the other sides of the domain.

## 4.3 Boundary Conditions

Boundary conditions for  $B$ -particle distribution functions, which are needed for simulations of flow and mass transfer problem in the structure, are presented. Boundary conditions for component  $A$  are the same as ones described in Chapter 3.

### On the Body

At the lattice node  $P$  on the body, shown in Figure 3.2, two types of boundary condition for component  $B$  are considered. One is the case that concentration of component  $B$  is given at the surface of the body, and the other is the case that normal mass flux of component  $B$  is constant at the surface. The distribution functions of component  $B$  such that  $\mathbf{c}_i \cdot \mathbf{n} > 0$  are unknown at the lattice node  $P$ . As in the case of single phase flow, when the concentration of component  $B$  is given at the node  $P$ , it is assumed that the unknown distribution functions have a similar form of the equilibrium distribution function given by Equation (2.4.10). In the following, the counter slip velocity which has two components at the node  $P$  is assumed to be zero for the same reason as described in Section 3.3. Then the unknown distribution

functions are expressed by

$$f_{Bi} = E_i \rho'_B \quad \text{for } \mathbf{c}_i \cdot \mathbf{n} > 0, \quad (4.3.1)$$

where  $\rho'_B$  is an unknown parameter. The unknown parameter is determined on the condition that the concentration of component  $B$  at the node  $P$  is equal to a given value  $\rho_B|_w$ . Substituting Equation (4.3.1) and the known distribution functions  $f_{Bi}$  for  $\mathbf{c}_i \cdot \mathbf{n} \leq 0$  into Equation (2.4.2) for  $\sigma = B$ , the unknown parameter  $\rho'_B$  is specified as follows:

$$\rho'_B = \frac{\rho_B|_w - \sum_{i(\mathbf{c}_i \cdot \mathbf{n} \leq 0)} f_{Bi}}{\sum_{i(\mathbf{c}_i \cdot \mathbf{n} > 0)} E_i}. \quad (4.3.2)$$

On the other hand, when normal mass flux of component  $B$  is constant value  $u_{Bn} (= \rho_B|_w u_{Bn})$  at the node  $P$ , the unknown distribution functions at the node  $P$  are also assumed to be Equation (4.3.1). In this case, substituting Equation (4.3.1) and the known distribution functions  $f_{Bi}$  for  $\mathbf{c}_i \cdot \mathbf{n} \leq 0$  into Equation (2.4.3) for  $\sigma = B$ , the unknown parameter  $\rho'_B$  is specified as follows:

$$\rho'_B = \frac{u_{Bn} - \sum_{i(\mathbf{c}_i \cdot \mathbf{n} \leq 0)} (\mathbf{c}_i \cdot \mathbf{n}) f_{Bi}}{\sum_{i(\mathbf{c}_i \cdot \mathbf{n} > 0)} (\mathbf{c}_i \cdot \mathbf{n}) E_i}. \quad (4.3.3)$$

### On the Side of Domain

On the sides of the domain except for the inlet and outlet, we assume that the normal flux of component  $B$  is equal to zero. Thus, the boundary condition on the body with constant mass flux is also applied to this case by setting the

constant value  $n_{Bn}$  in Equation (4.3.3) to be zero. For example, at the lattice node on the face CDHG in Figure 3.1, we express the unknown distribution functions  $f_{B3}$ ,  $f_{B8}$ ,  $f_{B9}$ ,  $f_{B11}$ , and  $f_{B14}$  by using Equation (4.3.1). The unknown parameter  $\rho'_B$  is given by Equation (4.3.3) for  $n_{Bn} = 0$ , i.e.,

$$\rho'_B = 6(f_{B6} + f_{B10} + f_{B12} + f_{B13} + f_{B15}). \quad (4.3.4)$$

On the corner line, e.g., on the line CG,  $f_{B3}$ ,  $f_{B4}$ ,  $f_{B8}$ ,  $f_{B9}$ ,  $f_{B10}$ ,  $f_{B11}$ ,  $f_{B14}$ , and  $f_{B15}$  are unknown distribution functions. In these unknowns, since  $f_{B10}$ ,  $f_{B11}$ ,  $f_{B14}$ , and  $f_{B15}$  are the distribution functions whose velocity points from the outer to outer region, one cannot determine the above-mentioned unknown distribution functions even though the line is regarded as a common part of the two faces. In the present calculations, all the distribution functions including known distribution functions on the CG are set to be averaged value of the corresponding distribution function at two nearest neighboring lattice nodes in the  $y$ - and  $z$ -directions. The same procedure is used on the other three corner lines and at every vertex from C through J.

### At the Inlet and Outlet

At the inlet and outlet, a periodic boundary condition is assumed. For given values of Reynolds and Schmidt numbers, the solution of the dimensionless concentration  $(\rho_B|_w - \rho_B)/(\rho_B|_w - \bar{\rho}_B|_{in})$ , where  $\bar{\rho}_B|_{in}$  is a time- and space-averaged concentration of component  $B$  at the inlet in each periodic section, can be uniquely obtained in every periodic section. However, the concentration of component  $B$  at the inlet is unknown quantity in advance. Thus, the concentration difference  $\Delta\rho_B$  between the inlet and outlet is specified.

The unknown distribution functions at the inlet and outlet are determined as follows. At the inlet, the unknown distribution functions are  $f_{B2}$ ,  $f_{B8}$ ,  $f_{B10}$ ,  $f_{B11}$ , and  $f_{B13}$ . Taking account of the form of the equilibrium distribution functions given by Equation (2.4.10) and neglecting the second- and higher-order terms of Knudsen number compared with the terms of  $O(1)$ , we assume that the unknown distribution functions at the inlet can be written by adding constant values to the corresponding known distribution functions at the outlet as follows:

$$f_{Bi}|_{in} = f_{Bi}|_{out} + E_i(K_1 + c_{ix}K_2 + c_{iy}K_3 + c_{iz}K_4) \quad \text{for } i = 2, 8, 10, 11, 13, \quad (4.3.5)$$

where  $K_1$ ,  $K_2$ ,  $K_3$ , and  $K_4$  are constants and  $c_{ix}$ ,  $c_{iy}$ , and  $c_{iz}$  are the  $x$ -,  $y$ -, and  $z$ -components of the velocity vector  $\mathbf{c}_i$ , respectively. Similarly, at the outlet, the unknown distribution functions  $f_{B5}$ ,  $f_{B9}$ ,  $f_{B12}$ ,  $f_{B14}$ , and  $f_{B15}$  are assumed to be written by subtracting constant values from the corresponding known distribution functions at the inlet:

$$f_{Bi}|_{out} = f_{Bi}|_{in} - E_i(K_1 + c_{ix}K_2 + c_{iy}K_3 + c_{iz}K_4) \quad \text{for } i = 5, 9, 12, 14, 15, \quad (4.3.6)$$

Then the constant values  $K_1$ ,  $K_2$ ,  $K_3$ , and  $K_4$  are determined by the following conditions. First, the concentration difference of component  $B$  between the inlet and outlet is equal to  $\Delta\rho_B (= \rho_B|_{out} - \rho_B|_{in})$ , that is,

$$\sum_{i=1}^{15} (f_{Bi}|_{out} - f_{Bi}|_{in}) = \Delta\rho_B. \quad (4.3.7)$$

Next, considering the boundary condition for component  $A$  at the inlet and outlet, we get

$$\sum_{i=1}^{15} c_{i\alpha} (f_{Bi}|_{\text{out}} - f_{Bi}|_{\text{in}}) = \Delta\rho_B u_{A\alpha}|_{\text{in}} \quad \text{for } \alpha = x, y, z, \quad (4.3.8)$$

where  $u_{A\alpha}|_{\text{in}}$  is the  $\alpha$ -component of the flow velocity of component  $A$  at the inlet. Therefore, we finally obtain four equations for four unknowns. The solutions are obtained as follows:

$$K_1 = 3 \left[ f_{B1}|_{\text{out}} - f_{B1}|_{\text{in}} + f_{B3}|_{\text{out}} - f_{B3}|_{\text{in}} + f_{B4}|_{\text{out}} - f_{B4}|_{\text{in}} + f_{B6}|_{\text{out}} - f_{B6}|_{\text{in}} + f_{B7}|_{\text{out}} - f_{B7}|_{\text{in}} - \Delta\rho_B \right], \quad (4.3.9)$$

$$K_2 = -3 \Delta\rho_B u_{Ax}|_{\text{in}}, \quad (4.3.10)$$

$$K_3 = 9 \left[ f_{B3}|_{\text{out}} - f_{B3}|_{\text{in}} - f_{B6}|_{\text{out}} + f_{B6}|_{\text{in}} - \Delta\rho_B u_{Ay}|_{\text{in}} \right], \quad (4.3.11)$$

$$K_4 = 9 \left[ f_{B4}|_{\text{out}} - f_{B4}|_{\text{in}} - f_{B7}|_{\text{out}} + f_{B7}|_{\text{in}} - \Delta\rho_B u_{Az}|_{\text{in}} \right]. \quad (4.3.12)$$

Substituting Equations (4.3.9)–(4.3.12) into Equations (4.3.5) and (4.3.6), all the unknown distribution functions for component  $B$  at the inlet and outlet are determined for the given  $\Delta\rho_B$ .

In addition, the unknown distribution functions on the corner lines of the inlet and outlet except for the vertices are calculated by the combination of the above-mentioned boundary conditions at the inlet and outlet and on the sides of the domain. For example, on the lines CF and GJ in Figure 3.1, taking account of the fact that  $u_{Az}=0$ , we first assume  $f_{B2}|_{\text{in}}$ ,  $f_{B11}|_{\text{in}}$ ,  $f_{B13}|_{\text{in}}$ ,  $f_{B5}|_{\text{out}}$ ,  $f_{B12}|_{\text{out}}$ , and  $f_{B14}|_{\text{out}}$  to be written by the following equations with constant values  $K_5$ ,  $K_6$ , and  $K_7$ :

$$f_{Bi}|_{\text{in}} = f_{Bi}|_{\text{out}} + E_i(K_5 + c_{ix}K_6 + c_{iy}K_7) \quad \text{for } i = 2, 11, 13, \quad (4.3.13)$$

$$f_{Bi}|_{\text{out}} = f_{Bi}|_{\text{in}} - E_i(K_5 + c_{ix}K_6 + c_{iy}K_7) \quad \text{for } i = 5, 12, 14, \quad (4.3.14)$$

Then, the other unknown distribution functions are expressed by using Equation (4.3.1) with parameters  $\rho'_B|_{\text{in}}$  and  $\rho'_B|_{\text{out}}$ . The unknown parameters are determined by Equations (4.3.7), (4.3.8) for  $\alpha = x, y$ , and (4.3.3) at the inlet and outlet. Hence, we obtain five equations for five unknowns. The solutions are given by

$$K_5 = 3 \left[ f_{B1}|_{\text{out}} - f_{B1}|_{\text{in}} + f_{B3}|_{\text{out}} - f_{B3}|_{\text{in}} + f_{B6}|_{\text{out}} - f_{B6}|_{\text{in}} + 2(f_{B7}|_{\text{out}} - f_{B7}|_{\text{in}}) - \Delta\rho_B \right], \quad (4.3.15)$$

$$K_6 = -\frac{18}{5} \Delta\rho_B u_{Ax}|_{\text{in}}, \quad (4.3.16)$$

$$K_7 = 18 \left[ f_{B3}|_{\text{out}} - f_{B3}|_{\text{in}} - f_{B6}|_{\text{out}} + f_{B6}|_{\text{in}} - \Delta\rho_B u_{Ay}|_{\text{in}} \right], \quad (4.3.17)$$

$$\rho'_B|_{\text{in}} = \frac{1}{6}(K_5 + K_6) + 6 \left[ f_{B7}|_{\text{in}} + f_{B11}|_{\text{out}} + f_{B12}|_{\text{in}} + f_{B13}|_{\text{out}} + f_{B14}|_{\text{in}} \right], \quad (4.3.18)$$

$$\rho'_B|_{\text{out}} = -\frac{1}{6}(K_5 - K_6) + 6 \left[ f_{B7}|_{\text{out}} + f_{B11}|_{\text{out}} + f_{B12}|_{\text{in}} + f_{B13}|_{\text{out}} + f_{B14}|_{\text{in}} \right], \quad (4.3.19)$$

The same method is used on the other corner lines of the inlet and outlet.

## 4.4 Computational Conditions

The computational domain is divided into  $73 \times 69 \times 69$  cubic lattice in the  $x$ -,  $y$ -, and  $z$ -directions. The Schmidt number  $Sc = \mu / (\bar{\rho}_A|_{in} D_{BA})$  is fixed at 0.1 in order to maintain numerical stability at high Reynolds numbers. The pressure difference of component  $A$  between the inlet and outlet and the viscosity of fluid  $A$  are changed so that the range of the Reynolds number  $Re = \bar{\rho}_A|_{in} \bar{u}_A|_{in} D_p / \mu$  is  $1.71 \leq Re \leq 105$ , where  $\bar{\rho}_A|_{in}(=1)$  and  $\bar{u}_A|_{in}$  are the time- and space-averaged density and velocity of component  $A$  at the inlet after transitional flows, respectively. The concentration difference of component  $B$  between the inlet and outlet is fixed at  $\Delta\rho_B = 0.2$ . The initial conditions for the velocity and density or concentration of components  $A$  and  $B$  are  $\mathbf{u}_A = \mathbf{u}_B = 0$ , and  $\rho_A = \rho_B = 1$  in the whole domain.

## 4.5 Results and Discussion

### 4.5.1 Flow Characteristics and Concentration Profiles

We first consider a mass transfer problem under the condition that  $B$ -species is diffused only from the center-located body  $M_B$  whose center is located at  $(x/L_x, y/L_y, z/L_z) = (0.48, 0.49, 0.49)$ . On the body  $M_B$  the concentration of component  $B$  is kept at constant value ( $\rho_B|_w = 3$ ), and on the other bodies normal mass flux of component  $B$  is zero. Figures 4.1–4.3 show the calculated results of velocity vectors of component  $A$  and concentration profiles of component  $B$  on the different planes ( $y/L_y = 0.36, 0.88$ , and  $x/L_x = 0.51$ ) for various Reynolds numbers after transitional flows. In these figures, the length of vectors is normalized so that the  $\bar{u}_A|_{in}$  has the same length in spite of different Reynolds numbers, and the bodies in the structure are depicted by the spheres with the equivalent diameter  $D_p = 29.4\Delta x$ . Note that in Figures 4.1 and 4.3 the center-located dark gray body represents the

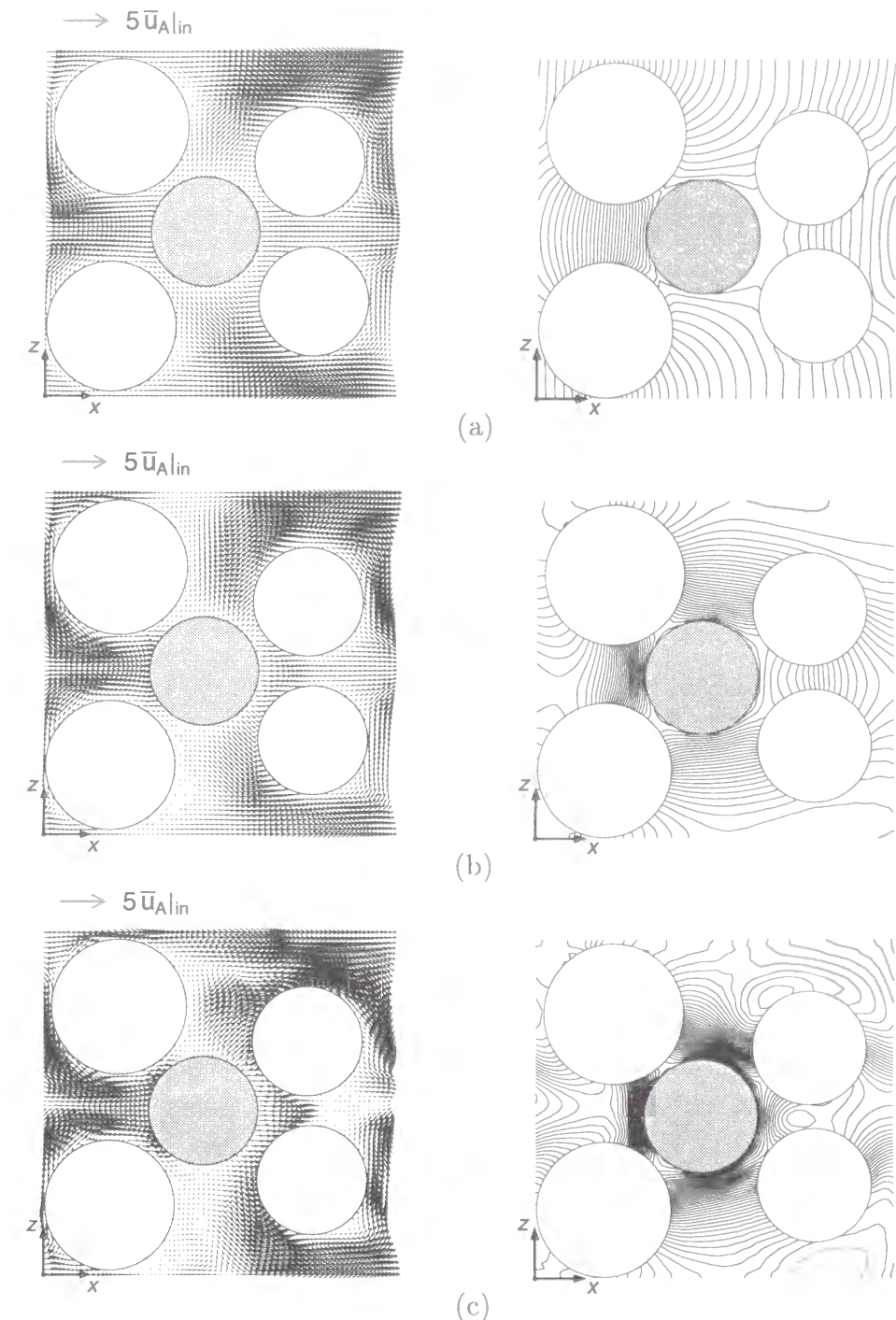


Figure 4.1: Velocity vectors of component  $A$  (left) and concentration profiles of component  $B$  (right) on the plane of  $y/L_y = 0.36$  at various Reynolds numbers: (a)  $Re = 1.71$ ,  $\delta\rho_B = 4.76 \times 10^{-3}$ ; (b)  $Re = 30.9$ ,  $\delta\rho_B = 1.23 \times 10^{-2}$ ; (c)  $Re = 105$ ,  $\delta\rho_B = 3.80 \times 10^{-2}$ , where  $\delta\rho_B$  is a contour interval. The center-located dark gray body is  $M_B$ .

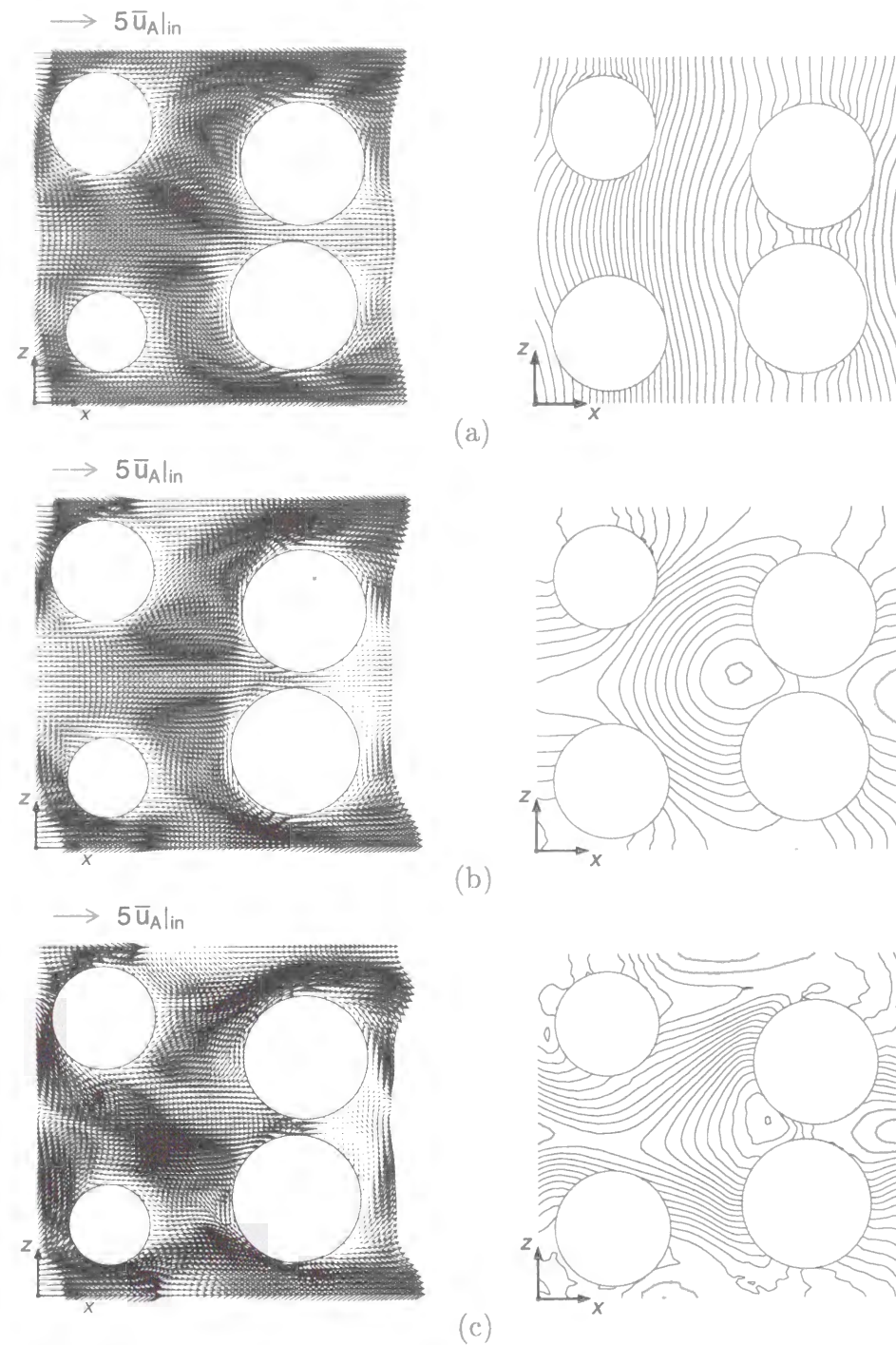


Figure 4.2: Velocity vectors of component A (left) and concentration profiles of component B (right) on the plane of  $y/L_y = 0.88$  at various Reynolds numbers: (a)  $Re = 1.71$ ,  $\delta\rho_B = 4.76 \times 10^{-3}$ ; (b)  $Re = 30.9$ ,  $\delta\rho_B = 1.23 \times 10^{-2}$ ; (c)  $Re = 105$ ,  $\delta\rho_B = 3.80 \times 10^{-2}$ , where  $\delta\rho_B$  is a contour interval. This plane has no cross-section of the body  $M_B$ .

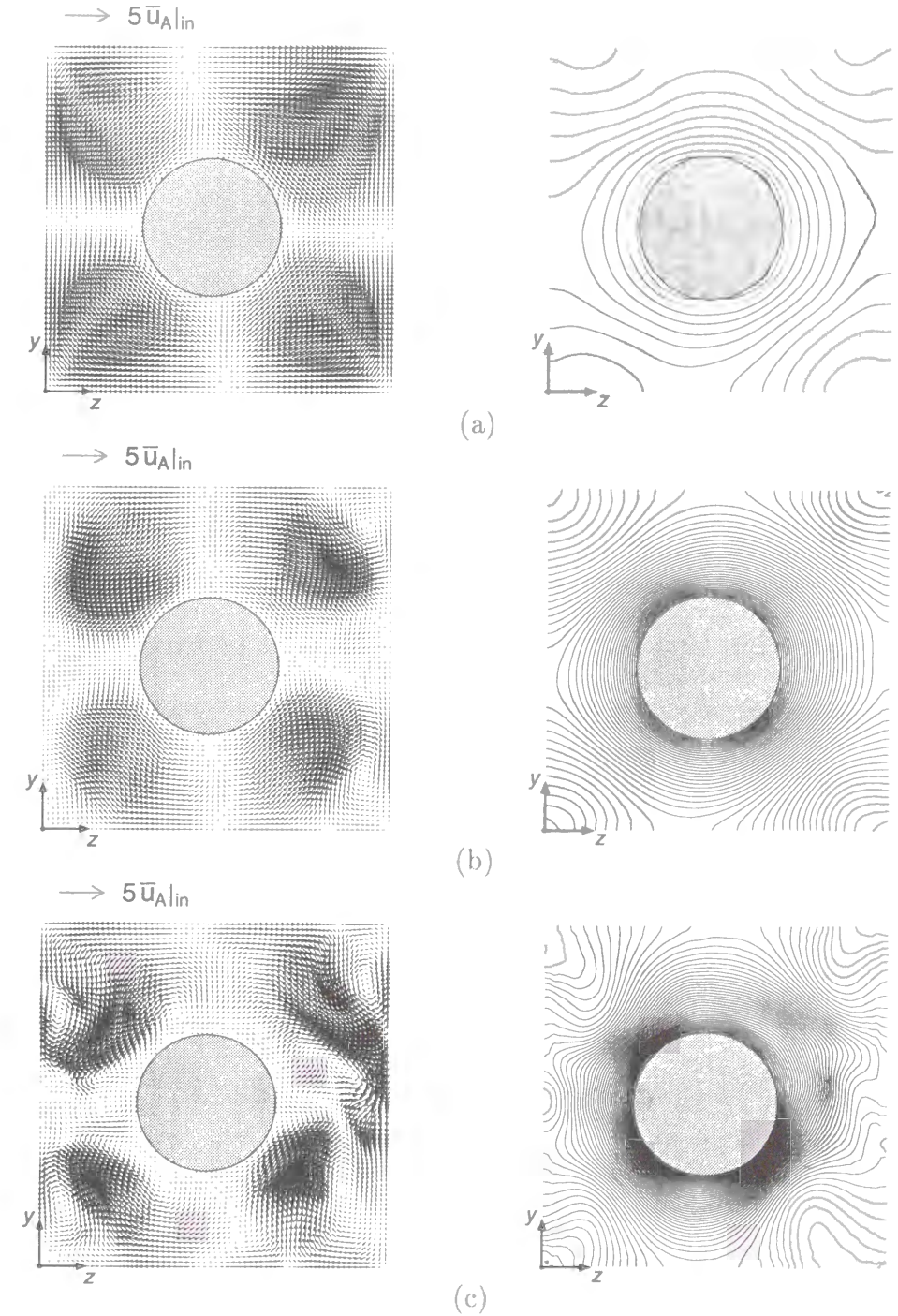


Figure 4.3: Velocity vectors of component A (left) and concentration profiles of component B (right) on the plane of  $x/L_x = 0.51$  at various Reynolds numbers: (a)  $Re = 1.71$ ,  $\delta\rho_B = 4.76 \times 10^{-3}$ ; (b)  $Re = 30.9$ ,  $\delta\rho_B = 1.23 \times 10^{-2}$ ; (c)  $Re = 105$ ,  $\delta\rho_B = 3.80 \times 10^{-2}$ , where  $\delta\rho_B$  is a contour interval. The dark gray body is  $M_B$ .

body  $M_B$  from which  $B$ -species is diffused. Figures 4.1 and 4.2 show the results on the two different planes parallel to the main flow. It is found from Figure 4.1 that at low Reynolds number of  $Re = 1.71$  the flow of component  $A$  avoids the bodies and goes through open spaces, and the concentration of component  $B$  increases almost linearly in the  $x$ -direction. Also, it is found from Figure 4.1(a) that the concentration gradient in front of the body  $M_B$  becomes large because of the diffusion of component  $B$  counter to the flow of component  $A$ . When  $Re = 30.9$ , on the other hand, it is seen that the flow speed becomes a little larger and component  $B$  is diffused together with flow of component  $A$ . At high Reynolds number of  $Re = 105$  the flow separations occur and weak vortices appear behind the bodies. In addition, the concentration of component  $B$  is highly affected by the convection of component  $A$ . Figure 4.2 shows the calculated results on the different plane parallel to main flow. It is noted that this plane has no cross-section of the body  $M_B$ . At low Reynolds number the concentration profiles of the component  $B$  is almost uniform vertical to main flow. On the contrary, at high Reynolds number, the component  $B$  diffuses mainly through the central region of the domain and is completely different from those at low Reynolds numbers. Figures 4.3 shows the results on the plane vertical to the main flow. It is seen from Figure 4.3 that at  $Re = 1.71$  the concentration of component  $B$  is almost uniform on the  $y$ - $z$  planes, while at  $Re = 105$  the steep concentration gradient exists around the body  $M_B$  and the concentration profile becomes more complicated. Finally, flow characteristics of component  $B$  around the body  $M_B$  are investigated. Figure 4.4 shows the mass flux vectors of component  $B$  on the planes  $y/L_y = 0.49$  and  $x/L_x = 0.48$  at low and high Reynolds numbers. It is noted that both planes intersect the center of the body  $M_B$ . At low Reynolds number component  $B$  is diffused in almost isotropic direction around the body  $M_B$ .

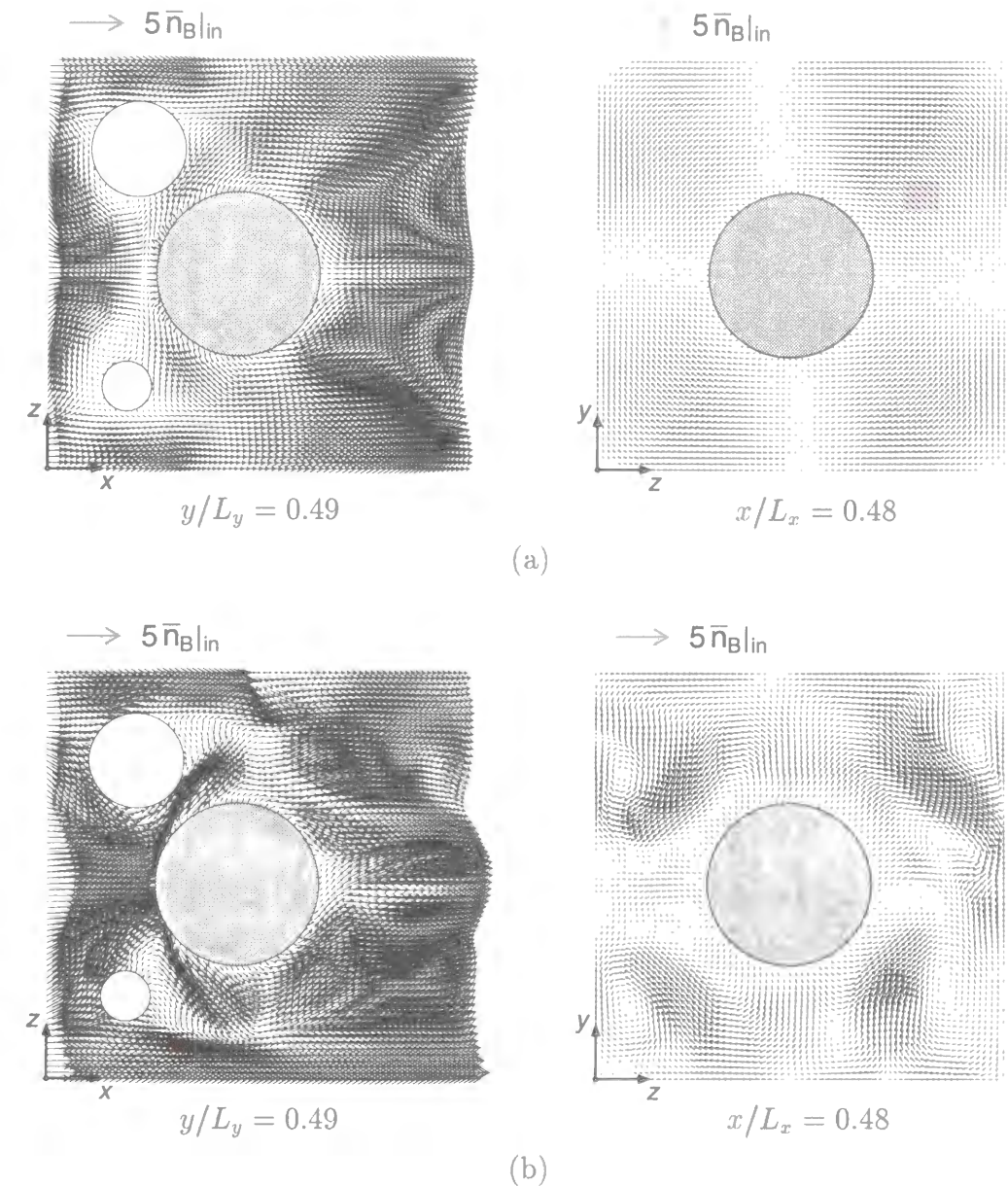


Figure 4.4: Mass flux vectors  $\mathbf{n}_B (= \rho_B \mathbf{u}_B)$  of component  $B$  on the planes of  $y/L_y = 0.49$  (left) and  $x/L_x = 0.48$  (right) at low and high Reynolds numbers: (a)  $Re = 1.71$ ,  $\bar{n}_B|_{in} = 1.45 \times 10^{-2}$ ; (b)  $Re = 105$ ,  $\bar{n}_B|_{in} = 1.05 \times 10^{-1}$ , where  $\bar{n}_B|_{in}$  is the time- and space-averaged  $x$ -component mass flux of component  $B$  at the inlet. The center-located dark gray body is  $M_B$ .

However, at high Reynolds number component  $B$  is much influenced by the approaching flow of component  $A$  in front of the body  $M_B$  and is carried downstream by the convection of component  $A$ . In addition, it is seen that the flow separation of component  $B$  occurs in the neighborhood of the body  $M_B$ . On the other hand, it is found that the mass flux of component  $B$  behind the body  $M_B$  is directly affected by the wake.

### 4.5.2 Sherwood Numbers

We next consider another mass transfer problem under the condition that  $B$ -species is diffused from all the bodies in the structure. In the following calculation, as an example of an ideal case, the concentration of component  $B$  at the lattice nodes on the bodies is changed linearly from the inlet through outlet so that the concentration difference of component  $B$  between the body and the fluid,  $\rho_B|_w - \rho_{Bm}$  ( $\rho_{Bm}$ : bulk concentration of component  $B$ ), can become equal value at the inlet and outlet under the periodic boundary condition. The other conditions are the same as the previous ones. The calculations are carried out for  $Re = 62.6, 79.0$ , and  $104$ . The averaged Sherwood number  $Sh_{av}$  is calculated by

$$Sh_{av} = \frac{\Delta \rho_B}{(\rho_B|_w - \rho_{Bm})_{in}} Re Sc \frac{L_y L_z}{S_{tot}}, \quad (4.5.1)$$

where  $S_{tot}$  is the total surface area of all the bodies in the structure and  $(\rho_B|_w - \rho_{Bm})_{in}$  is the bulk concentration difference of component  $B$  between the bodies and the inlet. Figure 4.5 shows the comparison of calculated results with experimental data with a low Schmidt number ( $Sc = 0.6$ ) for packed beds (Petrovic & Thodos 1968). It is found from this figure that the calculated values of  $Sh_{av} Sc^{-1/3}$  agree with the experimental data, although a little larger especially at the low Reynolds number.

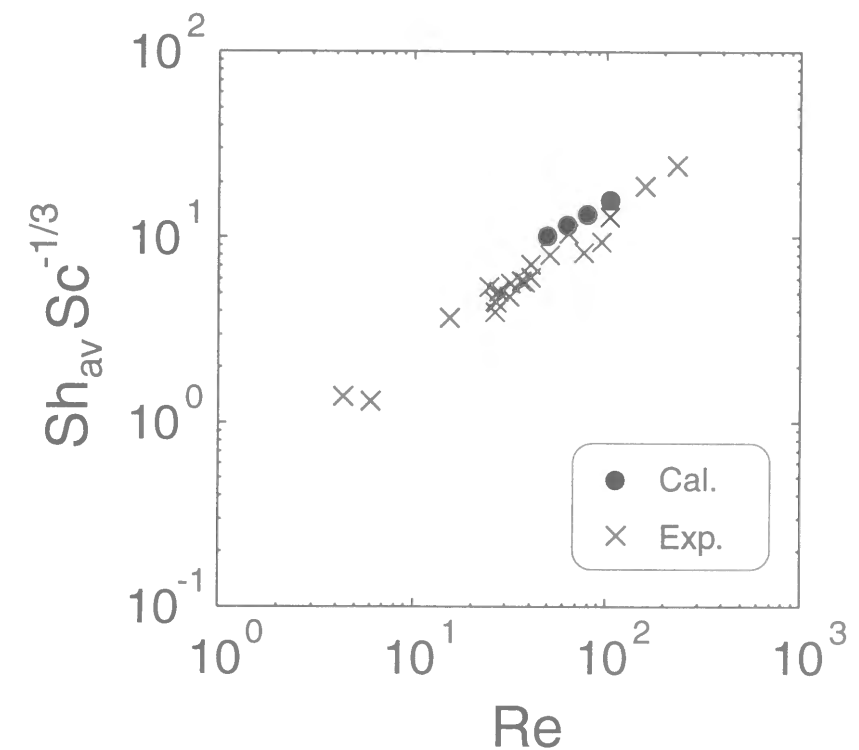


Figure 4.5: Comparison of calculated Sherwood numbers with experimental data: ●, the present calculated results; ×, the experimental data by Petrovic & Thodos.

## 4.6 Concluding Remarks

The LBM for a binary fluid mixture is applied to the problem of flow and mass transfer in a three-dimensional porous structure. Qualitatively reasonable results for concentration profiles are obtained for various Reynolds numbers. In addition, Sherwood numbers are calculated and compared with the experimental data for packed beds by Petrovic & Thodos. The results indicate that the calculated Sherwood numbers are in agreement with the experimental data. Finally, it should be noted that by taking advantage of the formal analogy between heat and mass transfer, the calculated concentration profiles and the Sherwood numbers can be regarded as temperature distributions and Nusselt numbers, respectively, in the analogous heat transfer problem. Therefore, the present method is useful for the investigation of microscopic properties of heat transfer as well as mass transfer in porous media.

# Chapter 5

## General Conclusion

### 5.1 Conclusion

In this thesis, numerical studies on fluid flow problems and flow and mass transfer problems in a three-dimensional porous structure are carried out by the lattice Boltzmann method (LBM). The transport phenomena in the structure are investigated from the microscopic point of view. From the whole results the following conclusions are obtained.

In Chapter 2, the fundamental theories of the LBM are discussed. First, the asymptotic theory proposed by Sone is applied to the LBM with the fifteen-velocity model and the continuity equation and the Navier-Stokes equations for incompressible fluid are derived. From the fluid-dynamic type equations of the LBM it is found that by using the LBM one can obtain the macroscopic flow velocities and the pressure gradient for incompressible fluid with relative errors of  $O(k^2)$  where  $k$  is a modified Knudsen number which is of the same order as the lattice spacing and is related to a dimensionless relaxation time. Next, a no-slip boundary condition at a wall and a periodic boundary condition at inlet and outlet are proposed. By calculating fundamental problems with these boundary conditions, it is found that the present methods are accurate to model the boundaries in physical systems. Finally,

the LBM for a binary fluid mixture with a simple kinetic model is proposed.

In Chapter 3, numerical studies on flows in a three-dimensional porous structure are carried out by using the LBM. Flow fields at a pore scale and pressure drops through the structure are calculated for various Reynolds numbers. From the comparison of the calculated pressure drops with empirical equations based on experimental data, it is found that the calculated pressure drops agree well with the empirical equations for low and high Reynolds numbers. Next, the characteristics of the unsteady flows in the transition region from laminar to turbulent flow are investigated. It is found that the Reynolds numbers where the velocity fluctuation begins and the transition from laminar and turbulent flow occurs depend on the positions in the structure.

In Chapter 4, numerical studies on flow and mass transfer in the porous structure are carried out by using the LBM for a binary fluid mixture. Flow characteristics and concentration profiles of diffusing component at a pore scale are obtained for various Reynolds numbers. At high Reynolds numbers concentration profiles are much affected by flow convection and become completely different from those at low Reynolds numbers. In addition, Sherwood numbers are calculated and compared with available experimental data for packed beds. The results indicate that the present method is useful for the microscopic studies of transport phenomena in porous structures.

## 5.2 Remarks for Further Studies

Finally, remarks and recommendation for further studies are given. In this thesis, numerical studies on heat transfer in the porous structure have not been discussed.

As mentioned in Chapter 4, by taking advantage of the formal analogy between heat and mass transfer, the results in the mass transfer problems can be viewed as those in the analogous heat transfer problems. However, when the problems of heat transfer in porous media are considered, it is often important to investigate heat transfer inside the bodies as well as in the fluid region. Besides, the problems of simultaneous heat/mass transfer and chemical reaction/diffusion systems in porous media are also attractive topics. Since the LBM has the advantages of the simplicity of the algorithm and flexibility for complex flows, it is highly expected that the LBM is capable of simulating these problems. Therefore, it is recommended to develop the LBM for these simulations and to analyze the transport phenomena in porous media.

In addition, the LBM has another advantage of the parallel algorithm because of its locality which is suited to parallel computers, although the author has not used these machines in this study. Thus, it is also recommended that high speed lattice Boltzmann simulations be performed by making use of up-to-date parallel computers.

# Appendix A

## Matrix Notation of Equation (2.2.30)

The inhomogeneous linear algebraic equation (2.2.30) can be written as

$$A\mathbf{f} = \mathbf{y}, \quad (\text{A.1})$$

with

$$A = \frac{1}{72} \begin{bmatrix} 56 & -8 & -8 & -8 & -8 & -8 & -8 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -16 & 40 & -8 & -8 & 16 & -8 & -8 & -4 & 2 & -4 & -4 & 2 & -4 & 2 & 2 \\ -16 & -8 & 40 & -8 & -8 & 16 & -8 & -4 & -4 & 2 & -4 & 2 & 2 & -4 & 2 \\ -16 & -8 & -8 & 40 & -8 & -8 & 16 & -4 & -4 & -4 & 2 & 2 & 2 & 2 & -4 \\ -16 & 16 & -8 & -8 & 40 & -8 & -8 & 2 & -4 & 2 & 2 & -4 & 2 & -4 & -4 \\ -16 & -8 & 16 & -8 & -8 & 40 & -8 & 2 & 2 & -4 & 2 & -4 & -4 & 2 & -4 \\ -16 & -8 & -8 & 16 & -8 & -8 & 40 & 2 & 2 & 2 & -4 & -4 & -4 & -4 & 2 \\ -16 & -32 & -32 & -32 & 16 & 16 & 16 & 62 & -4 & -4 & -4 & 8 & 2 & 2 & 2 \\ -16 & 16 & -32 & -32 & -32 & 16 & 16 & -4 & 62 & 2 & 2 & 2 & 8 & -4 & -4 \\ -16 & -32 & 16 & -32 & 16 & -32 & 16 & -4 & 2 & 62 & 2 & 2 & -4 & 8 & -4 \\ -16 & -32 & -32 & 16 & 16 & 16 & -32 & -4 & 2 & 2 & 62 & 2 & -4 & -4 & 8 \\ -16 & 16 & 16 & 16 & -32 & -32 & -32 & 8 & 2 & 2 & 2 & 62 & -4 & -4 & -4 \\ -16 & -32 & 16 & 16 & 16 & -32 & -32 & 2 & 8 & -4 & -4 & -4 & 62 & 2 & 2 \\ -16 & 16 & -32 & 16 & -32 & 16 & -32 & 2 & -4 & 8 & -4 & -4 & 2 & 62 & 2 \\ -16 & 16 & 16 & -32 & -32 & -32 & 16 & 2 & -4 & -4 & 8 & -4 & 2 & 2 & 62 \end{bmatrix}. \quad (\text{A.2})$$

where

$$\mathbf{f} = [f_1^{(m)}, f_2^{(m)}, f_3^{(m)}, f_4^{(m)}, f_5^{(m)}, f_6^{(m)}, f_7^{(m)}, f_8^{(m)}, f_9^{(m)}, f_{10}^{(m)}, f_{11}^{(m)}, f_{12}^{(m)}, f_{13}^{(m)}, f_{14}^{(m)}, f_{15}^{(m)}]^T$$

with  $m \geq 1$ . (A.3)

and

$$\mathbf{y} = [Ih_1^{(m)}, Ih_2^{(m)}, Ih_3^{(m)}, Ih_4^{(m)}, Ih_5^{(m)}, Ih_6^{(m)}, Ih_7^{(m)}, Ih_8^{(m)},$$

$$Ih_9^{(m)}, Ih_{10}^{(m)}, Ih_{11}^{(m)}, Ih_{12}^{(m)}, Ih_{13}^{(m)}, Ih_{14}^{(m)}, Ih_{15}^{(m)}]^T$$

with  $m \geq 1$ . (A.4)

It is easily verified that  $\text{rank}(A^T) = 11$  and the homogeneous equation  $A^T \mathbf{f}' = \mathbf{0}$  has the following four nontrivial solutions:

$$\mathbf{f}' =$$

$$[2/9, 1/9, 1/9, 1/9, 1/9, 1/9, 1/9, 1/72, 1/72, 1/72, 1/72, 1/72, 1/72, 1/72, 1/72]^T,$$

$$[0, 1/9, 0, 0, -1/9, 0, 0, 1/72, -1/72, 1/72, 1/72, -1/72, 1/72, -1/72, -1/72]^T,$$

$$[0, 0, 1/9, 0, 0, -1/9, 0, 1/72, 1/72, -1/72, 1/72, -1/72, -1/72, 1/72, -1/72]^T,$$

and

$$[0, 0, 0, 1/9, 0, 0, -1/9, 1/72, 1/72, 1/72, -1/72, -1/72, -1/72, -1/72, 1/72]^T.$$

It should be noted that the elements of the four nontrivial solution vectors are  $E_i$ ,  $E_i \hat{c}_{i1}$ ,  $E_i \hat{c}_{i2}$ , and  $E_i \hat{c}_{i3}$ , respectively.

## Appendix B

### Solvability Conditions of Linear Algebraic Equations

Consider linear algebraic equations

$$A\mathbf{f} = \mathbf{y}. \quad (\text{B.1})$$

If the ‘transposed’ homogeneous linear algebraic equations

$$A^T \mathbf{f}' = \mathbf{0} \quad (\text{B.2})$$

has a positive number  $r$  of nontrivial (not identically zero) linearly independent solutions,  $\mathbf{f}'_1, \mathbf{f}'_2, \dots, \mathbf{f}'_r$ , then the solvability conditions of linear algebraic Equation (B.1) are

$$\mathbf{f}'_j \cdot \mathbf{y} = 0 \quad \text{for } j = 1, 2, \dots, r. \quad (\text{B.3})$$

This means that Equation (B.1) has solutions if and only if  $\mathbf{y}$  is orthogonal to every nontrivial solution  $\mathbf{f}'$  of Equation (B.2).

## Nomenclature

|                                          |                                                                          |                                    |
|------------------------------------------|--------------------------------------------------------------------------|------------------------------------|
| $A$                                      | coefficient matrix of linear algebraic equations                         | $[-]$                              |
| $A_c$                                    | constant coefficient in collision term                                   | $[-]$                              |
| $\mathbf{b}$                             | unit vector perpendicular to $\mathbf{n}$                                | $[-]$                              |
| $c$                                      | characteristic particle speed                                            | $[\text{m/s}]$                     |
| $\bar{c}$                                | mean particle speed                                                      | $[\text{m/s}]$                     |
| $c_0$                                    | speed of sound                                                           | $[\text{m/s}]$                     |
| $\mathbf{c}_i, \mathbf{c}_i$             | particle velocities                                                      | $[\text{m/s}]$ or $[-]$            |
| $D$                                      | number of dimensional space                                              | $[-]$                              |
| $D_{BA}$                                 | diffusivity in binary fluid mixture                                      | $[-]$                              |
| $D_p$                                    | equivalent diameter of body                                              | $[-]$                              |
| $E_i$                                    | constant coefficients                                                    | $[-]$                              |
| $Er_1, Er_2$                             | error norms                                                              | $[-]$                              |
| $e, \hat{e}$                             | internal energy per unit mass                                            | $[\text{m}^2/\text{s}^2]$ or $[-]$ |
| $e_A$                                    | internal energy of component $A$ per unit mass                           | $[\text{m}^2/\text{s}^2]$ or $[-]$ |
| $F$                                      | frequency                                                                | $[-]$                              |
| $\mathbf{f}$                             | solution vector of linear algebraic equations                            | $[-]$                              |
| $\mathbf{f}'$                            | nontrivial solution of transposed homogeneous linear algebraic equations | $[-]$                              |
| $f_i, \hat{f}_i$                         | particle distribution functions                                          | $[\text{kg}/\text{m}^3]$ or $[-]$  |
| $f_i^{\text{eq}}, \hat{f}_i^{\text{eq}}$ | local equilibrium distribution functions                                 | $[\text{kg}/\text{m}^3]$ or $[-]$  |
| $f_{\sigma i}$                           | particle distribution functions for $\sigma$ -species                    | $[-]$                              |

|                             |                                                                                |             |
|-----------------------------|--------------------------------------------------------------------------------|-------------|
| $f_{A\sigma i}^{\text{eq}}$ | local equilibrium distribution functions for $\sigma$ -species                 | [—]         |
| $I_x$                       | turbulence intensity, $\sqrt{(\bar{u}_x - \bar{u}_x)^2} / \bar{u}_{\text{in}}$ | [—]         |
| $h_i^{(m)}$                 | inhomogeneous term of linear algebraic equations                               | [—]         |
| Kn                          | Knudsen number, $c/(A_c \rho_0 L)$                                             | [—]         |
| $k$                         | modified Knudsen number                                                        | [—]         |
| $L$                         | characteristics length                                                         | [m]         |
| $L_x, L_y, L_z$             | lengths of domain                                                              | [—]         |
| $M_B$                       | body from which $B$ -species is diffused                                       |             |
| Ma                          | Mach number, $U/c$                                                             | [—]         |
| $N$                         | number of particles                                                            | [—]         |
| $\mathbf{n}$                | unit normal vector                                                             | [—]         |
| $\mathbf{n}_B$              | mass flux of component $B$ , $\rho_B \mathbf{u}_B$                             | [—]         |
| P                           | boundary lattice node                                                          |             |
| $P_1, P_2, P_3$             | points in porous structure                                                     |             |
| $p, p$                      | pressure                                                                       | [Pa] or [—] |
| $p_A$                       | pressure of component $A$                                                      | [—]         |
| Re                          | Reynolds number, $\rho_0 U L / \mu$                                            | [—]         |
| $\text{Re}'$                | modified Reynolds number, $\text{Re}/(1 - \varepsilon)$                        | [—]         |
| $S$                         | tangent plane on lattice node                                                  |             |
| $S_{\text{tot}}$            | total surface area of all the bodies                                           | [—]         |
| Sc                          | Schmidt number, $\mu/(\bar{\rho}_A _{\text{in}} D_{BA})$                       | [—]         |
| Sh                          | Strouhal number, $L/(t_0 c)$                                                   | [—]         |
| $\text{Sh}_{\text{av}}$     | Sherwood number                                                                | [—]         |
| St                          | Strouhal number, $FL_x/\bar{u}_{\text{in}}$                                    | [—]         |
| $\mathbf{t}$                | unit vector perpendicular to $\mathbf{n}$                                      | [—]         |
| $t, \hat{t}$                | time                                                                           | [s] or [—]  |

|                          |                                                                  |              |
|--------------------------|------------------------------------------------------------------|--------------|
| $t_0$                    | characteristic time scale, $L/U$                                 | [s]          |
| $U$                      | characteristic flow speed                                        | [m/s]        |
| $\mathbf{u}, \mathbf{u}$ | flow velocity                                                    | [m/s] or [—] |
| $\mathbf{u}_\sigma$      | flow velocity of component $\sigma$                              | [—]          |
| $u, v, w$                | $x$ -, $y$ -, and $z$ -components of flow velocity               | [—]          |
| $u_{Bn}$                 | normal flow velocity of component $B$                            | [—]          |
| $u_s$                    | slip velocity at wall                                            | [—]          |
| $\bar{u}_A _{\text{in}}$ | time- and space-averaged flow velocity of component $A$ at inlet | [—]          |
| $\bar{u}_{\text{in}}$    | time- and space-averaged flow velocity at inlet                  | [—]          |
| $\bar{u}_x$              | time-averaged value of $x$ -component of flow velocity           | [—]          |
| $\bar{u}'$               | space-averaged value of counter slip velocity                    | [—]          |
| $\mathbf{x}, \mathbf{x}$ | position vector                                                  | [m] or [—]   |
| $x_\alpha, x_\alpha$     | Cartesian coordinates, $(x_1, x_2, x_3)$ or $(x, y, z)$          | [—]          |
| $\mathbf{y}$             | inhomogeneous vector of linear algebraic equations               | [—]          |

### Greek Symbols

|                            |                                                                    |               |
|----------------------------|--------------------------------------------------------------------|---------------|
| $\Delta p$                 | pressure difference between inlet and outlet                       | [—]           |
| $\Delta t, \Delta \hat{t}$ | time step                                                          | [s] or [—]    |
| $\Delta x, \Delta \hat{x}$ | lattice spacing                                                    | [m] or [—]    |
| $\Delta \rho_B$            | concentration difference of component $B$ between inlet and outlet | [—]           |
| $\delta \rho_B$            | concentration contour interval of component $B$                    | [—]           |
| $\epsilon$                 | dimensionless number of the same order as Kn, $c/(A_c \rho_0 L)$   | [—]           |
| $\varepsilon$              | porosity                                                           | [—]           |
| $\mu, \hat{\mu}$           | fluid viscosity                                                    | [Pa·s] or [—] |

|                        |                                                                                                  |                                   |
|------------------------|--------------------------------------------------------------------------------------------------|-----------------------------------|
| $\Pi_B$                | dimensionless concentration of component $B$ ,<br>$(\rho_B - \rho_{B0})/(\rho_{B1} - \rho_{B0})$ | $[-]$                             |
| $\rho, \hat{\rho}$     | fluid density                                                                                    | $[\text{kg}/\text{m}^3]$ or $[-]$ |
| $\rho_A$               | density of component $A$                                                                         | $[-]$                             |
| $\rho_B$               | concentration of component $B$                                                                   | $[-]$                             |
| $\rho_{B\text{in}}$    | bulk concentration of component $B$                                                              | $[-]$                             |
| $\rho_B _w$            | concentration of component $B$ at wall                                                           | $[-]$                             |
| $\rho_{B0}, \rho_{B1}$ | constant concentration of component $B$                                                          | $[-]$                             |
| $\rho_w$               | density at wall                                                                                  | $[-]$                             |
| $\rho_0$               | reference density                                                                                | $[\text{kg}/\text{m}^3]$          |
| $\rho_A _{\text{in}}$  | time- and space-averaged fluid density of component $A$ at inlet                                 | $[-]$                             |
| $\rho_B _{\text{in}}$  | time- and space-averaged concentration of component $B$ at inlet                                 | $[-]$                             |
| $\rho_{\text{in}}$     | time- and space-averaged fluid density at inlet                                                  | $[-]$                             |
| $\tau$                 | single relaxation time                                                                           | $[-]$                             |
| $\tau_\sigma$          | single relaxation time for $\sigma$ -species                                                     | $[-]$                             |

**Overlines**

|                          |                 |
|--------------------------|-----------------|
| $\overline{\phantom{x}}$ | averaged        |
| $\bar{\phantom{x}}$      | non-dimensional |

**Subscripts**

|     |                                       |
|-----|---------------------------------------|
| $A$ | component $A$                         |
| $B$ | component $B$                         |
| av  | averaged                              |
| $i$ | $i$ th direction of particle velocity |

|           |                                   |
|-----------|-----------------------------------|
| in        | inlet                             |
| m         | bulk or mixing                    |
| n         | normal                            |
| $n, t, b$ | $n$ -, $t$ -, and $b$ -components |
| out       | outlet                            |
| s         | slip                              |
| w         | wall                              |
| $x, y, z$ | $x$ -, $y$ -, and $z$ -components |
| $\sigma$  | $\sigma$ -species                 |

**Superscripts**

|       |              |
|-------|--------------|
| eq    | equilibrium  |
| $(m)$ | $m$ th order |
| *     | analytical   |

# References

- Abe, T. 1997 Derivation of the lattice Boltzmann method by means of the discrete ordinate method for the Boltzmann equation. *J. Comput. Phys.* **131**, 241–246.
- Aidun, C. K. & Lu, Y. 1995 Lattice Boltzmann simulation of solid particles suspended in fluid. *J. Stat. Phys.* **81**, 49–61.
- Benzi, R., Struglia, M. V. & Tripiccone, R. 1996 Extended self-similarity in numerical simulations of three-dimensional anisotropic turbulence. *Phys. Rev. E* **53**, R5565–5568.
- Bhatnagar, P. L., Gross, E. P. & Krook, M. 1954 A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems. *Phys. Rev.* **94**, 511–525.
- Bird, R. B., Stewart, W. E. & Lightfoot, E. N. 1960 *Transport Phenomena*, pp. 196–200. John Wiley & Sons, New York.
- Broadwell, J. E. 1964 Study of rarefied shear flow by the discrete velocity method. *J. Fluid Mech.* **19**, 401–414.
- Buonanno, G. & Carotenuto, A. 1997 The effective thermal conductivity of a porous medium with interconnected particles. *Int. J. Heat Mass Transfer* **40**,

- 393–405.
- Cali, A., Succi, S., Cancelliere, A. & Benzi, R. & Gramignani, M. 1992 Diffusion and hydrodynamic dispersion with the lattice Boltzmann method. *Phys. Rev. A* **45**, 5771–5774.
- Cancelliere, A., Chang, C., Foti, E., Rothman, D. H. & Succi, S. 1990 The permeability of a random medium: comparison of simulation with theory. *Phys. Fluids A* **2**, 2085–2088.
- Chen, H., Chen, S. & Matthaeus, W. H. 1992 Recovery of the Navier–Stokes equations using a lattice-gas Boltzmann method. *Phys. Rev. A* **45**, R5339–5342.
- Chen, S., Chen, H., Martinez, D. & Matthaeus, W. H. 1991a Lattice Boltzmann model for simulation of magnetohydrodynamics. *Phys. Rev. Lett.* **67**, 3776–3779.
- Chen, S., Diemer, K., Doolen, G. D., Eggert, K., Fu, C., Gutman, S. & Travis, B. J. 1991b Lattice gas automata for flow through porous media. *Physica D* **47**, 72–84.
- Chen, S., Dawson, S. P., Doolen, G. D., Janecky, D. R. & Lawniczak, A. 1995 Lattice methods and their applications to reacting systems. *Comp. Chem. Eng.* **19**, 617–646.
- Chen, S. & Doolen, G. D. 1998 Lattice Boltzmann method for fluid flows. *Annu. Rev. Fluid Mech.* **30**, 329–364.

- Chen, Y., Ohashi, H. & Akiyama, M. 1997 Two-parameter thermal lattice BGK model with a controllable Prandtl number. *J. Sci. Comput.* **12**, 169–185.
- Courant, R. & Hilbert, D. 1953 *Methods of Mathematical Physics*, Vol. 1, Interscience, New York.
- Dawson, S. P., Chen, S. & Doolen, G. D. 1993 Lattice Boltzmann computations for reaction-diffusion equations. *J. Chem. Phys.* **98**, 1514–1523.
- d'Humières, D., Lallemand, P. & Frisch, U. 1986 Lattice gas model for 3D hydrodynamics. *Europhys. Lett.* **2**, 291–297.
- d'Humières, D. & Lallemand, P. 1987 Numerical simulations of hydrodynamics with lattice gas automata in two dimensions. *Complex Syst.* **1**, 599–632.
- Dybbs, A. & Edwards, R. V. 1984 A new look at porous media fluid mechanics — Darcy to turbulent. In *Fundamentals of Transport Phenomena in Porous Media* (eds. J. Bear & M. Y. Corapcioglu), pp. 199–256. Martinus Nijhoff Publishers, Dordrecht.
- Ergun, S. 1952 Fluid flow through packed columns. *Chem. Eng. Prog.* **48**, 89–94.
- Fand, R. M., Kim, B. Y. K., Lam, A. C. C. & Phan, R. T. 1987 Resistance to the flow of fluids through simple and complex porous media whose matrices are composed of randomly packed spheres. *Trans. ASME* **109**, 268–274.
- Ferziger, J. H. & Perić, M. 1996 *Computational Methods for Fluid Dynamics*. Springer, New York.

- Frisch, U., Hasslacher, B. & Pomeau, Y. 1986 Lattice-gas automata for the Navier–Stokes equations. *Phys. Rev. Lett.* **56**, 1505–1508.
- Frisch, U., d'Humières, D., Hasslacher, B., Lallemand, P., Pomeau, Y. & Rivert, J.-P. 1987 Lattice gas hydrodynamics in two and three dimensions. *Complex Syst.* **1**, 649–707.
- Garzó, V., Santos, A. & Brey, J. J. 1992 A kinetic model for a multicomponent gas. *J. Phys. Fluids A* **1**, 380–383.
- Ginzbourg, I. & Adler, P. M. 1994 Boundary flow condition analysis for the three-dimensional lattice Boltzmann model. *J. Phys. II France* **4**, 191–214.
- Gunstensen, A. K., Rothman, D. H., Zaleski, S. & Zanetti, G. 1991 Lattice Boltzmann model of immiscible fluids. *Phys. Rev. A* **43**, 4320–4327.
- He, X. & Luo, L.-S. 1997 A priori derivation of the lattice Boltzmann equation. *Phys. Rev. E* **55**, 6333–6336.
- He, X., Chen, S. & Doolen, G. D. 1998 A novel thermal model for the lattice Boltzmann method in incompressible limit. *J. Comput. Phys.* **146**, 282–300.
- He, X., Chen, S. & Doolen, G. D. 1999 Recent advances in the lattice Boltzmann method for multiphase flow. In *Research into application of microscopic fluid simulation to macroscopic systems*, pp. 55–103. Atomic Energy Society of Japan.
- Higuera, F. & Jimenez, J. 1989 Boltzmann approach to lattice gas simulations. *Europhys. Lett.* **9**, 663–668.

- Holme, R. & Rothman, D. H. 1992 Lattice-gas and lattice-Boltzmann methods of miscible fluids. *J. Stat. Phys.* **68**, 409–429.
- Hou, S., Zou, Q., Chen, S., Doolen, G. & Cogley, A. 1995 Simulation of cavity flow by the lattice Boltzmann method. *J. Comput. Phys.* **118**, 329–347.
- Hsu, C. T. & Cheng, P. 1990 Thermal dispersion in a porous medium. *Int. J. Heat Mass Transfer* **33**, 1587–1597.
- Inamuro, T. & Sturtevant B. 1990 Numerical study of discrete-velocity gases. *Phys. Fluids* **2**, 2196–2203.
- Inamuro, T., Yamamura, M. & Ogino, F. 1995 Lattice Boltzmann simulation of flow and heat transfer in a two-dimensional porous structure. In *Numerical Methods in Laminar and Turbulent Flow* (eds. C. Taylor & P. Durbetaki), Vol. 9, pp. 632–643. Pineridge Press, Swansea.
- Inamuro, T., Konishi, N. & Ogino, F. 1999 A Galilean invariant model of the lattice Boltzmann method for multiphase fluid flows using free-energy approach. *Comput. Phys. Commun.* in press.
- Inamuro, T., Miyahara, T. & Ogino, F. 2000 Lattice Boltzmann simulations of drop deformation and breakup in simple shear flows, in preparation.
- Kadanoff, L. 1986 On two levels. *Phys. Today* **39**, 7–9.
- Koch, D. L. & Brady, J. F. 1985 Dispersion in fixed beds. *J. Fluids Mech.* **154**, 399–427.

- Koplik, J. & Lasseter, T. 1984 One- and two-phase flow in network models of porous media. *Chem. Eng. Commun.* **26**, 285–295.
- Ladd, A. J. C. 1994 Numerical simulations of particulate suspensions via a discretized Boltzmann equation. *J. Fluid Mech.* **271**, 285–309, 310–339.
- Ladd, A. J. C. 1997 Sedimentation of homogeneous suspensions of non-Brownian spheres. *J. Phys. Fluids* **9**, 491–499.
- Liu, S., Afacan, A. & Masliyah, J. 1994 Steady incompressible laminar flow in porous media. *Chem. Eng. Sci.* **49**, 3565–3586.
- Maier, R. S., Bernard, R. S. & Gruman, D. W. 1996 Boundary conditions for the lattice Boltzmann method. *Phys. Fluids* **8**, 1778–1801.
- Martínez, D. O., Matthaeus, W. H., Chen, S. & Montgomery, D. C. 1994 Comparison of spectral method and lattice Boltzmann simulations of two-dimensional hydrodynamics. *Phys. Fluids* **6**, 1285–1298.
- McNamara, G. R., Garcia, A. L. & Alder, B. J. 1997 A hydrodynamically correct thermal lattice Boltzmann model. *J. Stat. Phys.* **87**, 1111–1121.
- McNamara, G. & Zanetti, G. 1988 Use of the lattice Boltzmann equation to simulate lattice-gas automata. *Phys. Rev. Lett.* **61**, 2332–2335.
- Noble, D. R., Chen, S., Geogiadis, J. G. & Buckins, R. O. 1995 A consistent hydrodynamic boundary condition for the lattice Boltzmann method. *Phys. Fluids* **7**, 203–209.

- Petrovic, L. & Thodos, G. 1968 Mass transfer in the flow of gases through packed beds. *Int. Eng. Chem. Fund.* **7**, 274–280.
- Qian, Y. H., d’Humières, D. & Lallemand, P. 1992 Lattice BGK models for Navier–Stokes equation. *Europhys. Lett.* **17**, 479–484.
- Reider, M. B. & Sterling, J. D. 1995 Accuracy of discrete-velocity BGK models for the simulation of the incompressible Navier–Stokes equations. *Comput. Fluids* **24**, 459–467.
- Rothman, D. H. 1988 Cellular-automaton fluids: a model for flow in porous media. *Geophys.* **54**, 509–518.
- Rothman, D. H. & Zaleski, S. 1997 *Lattice-Gas Cellular Automata*. Cambridge University Press.
- Schwarz, L. M., Martys, N., Bentz, D. P., Garboczi, E. J. & Torquato, S. 1993 Cross-property relations and permeability estimation in model porous media. *Phys. Rev. E* **48**, 4584–4591.
- Shan, X. & Chen, H. 1994 Simulation of non-ideal gases and liquid-gas phase transitions by the lattice Boltzmann equation. *Phys. Rev. E* **49**, 2941–2948.
- Shan, X. 1997 Simulation of Rayleigh–Bénard convection using a lattice Boltzmann method. *Phys. Rev. E* **55**, 2780–2788.
- Skordos, P. A. 1993 Initial and boundary conditions for the lattice Boltzmann method. *Phys. Rev. E* **48**, 4823–4842.

- Sone, Y. 1971 Asymptotic theory of flow of rarefied gas over a smooth boundary II. In *Rarefied Gas Dynamics* (ed. D. Dini), Vol. 2, pp. 737–749. Editrice Tecnico Scientifica, Pisa.
- Sone, Y. 1991 Asymptotic theory of a steady flow of a rarefied gas past bodies for small Knudsen numbers. In *Advances in Kinetic Theory and Continuum Mechanics* (eds. R. Gatignol & Soubbaramayer), pp. 19–31. Springer-Verlag, Berlin.
- Sone, Y. & Aoki, K. 1994 *Molecular Gas Dynamics*. Asakura, Tokyo (in Japanese).
- Spaid, M. A. A. & Phelan, F. R. 1997 Lattice Boltzmann methods for modeling microscale flow in fibrous porous media. *Phys. Fluids* **9**, 2468–2474.
- Sterling, J. D. & Chen, S. 1996 Stability analysis of lattice Boltzmann methods. *J. Comput. Phys.* **123**, 196–206.
- Strang, G. 1976 *Linear Algebra and Its Applications*. Academic Press, Inc., New York.
- Succi, S., Foti, E. & Higuera, F. 1989 Three-dimensional flows in complex geometries with the lattice Boltzmann method. *Europhys. Lett.* **10**, 433–438.
- Swift, M. R., Osborn, W. R. & Yeomans, J. M. 1995 Lattice Boltzmann simulation of nonideal fluids. *Phys. Rev. Lett.* **75**, 830–833.
- Swift, M. R., Orlandini, S. E., Osborn, W. R. & Yeomans, J. M. 1996 Lattice Boltzmann simulations of liquid-gas and binary-fluid systems. *Phys. Rev. E* **54**, 5041–5052.

- Tsutahara, M., Takada, N. & Kataoka, T. 1999 *Lattice Gas and Lattice Boltzmann Methods — New Methods of Computational Fluid Dynamics.* Corona, Tokyo (in Japanese).
- Wolfram, S. 1986 Cellular automaton fluids I: Basic theory. *J. Stat. Phys.* **45**, 471–526.
- Ziegler, D. P. 1993 Boundary conditions for lattice Boltzmann simulations. *J. Stat. Phys.* **71**, 1171–1177.
- Zou, Q., Hou, S., Chen, S. & Doolen, G. D. 1995 An improved incompressible lattice Boltzmann model for time-independent flows. *J. Stat. Phys.* **81**, 35–49.
- Zou, Q. & He, X. 1997 On pressure and velocity boundary conditions for the lattice Boltzmann BGK model. *Phys. Fluids* **9**, 1591–1598.

## List of Publications

### Journal

- [1] Inamuro, T., Yoshino, M. & Ogino, F. 1995 A non-slip boundary condition for lattice Boltzmann simulations. *Phys. Fluids* **7**, 2928–2930; Erratum **8**, 1124.
- [2] Inamuro, T., Yoshino, M. & Ogino, F. 1997 Accuracy of the lattice Boltzmann method for small Knudsen number with finite Reynolds number. *Phys. Fluids* **9**, 3535–3542.
- [3] Inamuro, T., Yoshino, M. & Ogino, F. 1999 Lattice Boltzmann simulation of flows in a three-dimensional porous structure. *Int. J. Numer. Meth. Fluids* **29**, 737–748.
- [4] Inamuro, T., Yoshino, M. & Ogino, F. 1999 Numerical analysis of unsteady flows in a three-dimensional porous structure. *Kagaku Kogaku Ronbunshu* **25**, 979–986 (in Japanese).
- [5] Inamuro, T., Inoue, H., Yoshino, M. & Ogino, F. 2000 Lattice Boltzmann simulation for binary fluid mixture, in preparation.

### International Conference

- [1] Inamuro, T., Yoshino, M. & Ogino, F. 1997 Lattice Boltzmann simulation of flows in a three-dimensional porous structure. In *Numerical Methods in Laminar and Turbulent Flow* (eds. C. Taylor & J. Cross), Vol. 10, pp. 129–140. Pineridge Press, Swansea.
- [2] Inamuro, T., Yoshino, M. & Ogino, F. 1998 Numerical analysis of unsteady flows in a porous structure by lattice Boltzmann method. In *Proc. 4th KSME JSME Fluids Eng. Conf.* (ed. M. J. Lee), pp. 245–248. Pusan.
- [3] Inamuro, T., Yoshino, M., Inoue, H. & Ogino, F. 1999 Lattice Boltzmann simulation of flow and mass transfer in a porous structure. In *Proc. 3rd Joint ASME–JSME Fluids Mech. Conf.* FEDSM99–6977. San Francisco.

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