Simulation of Flow in Complex Geometries by Immersed Boundary Method

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Simulation plays a critical role in the design of chemical equipment and the optimization of process conditions, as it enables the analysis of physical quantities distributed in three dimensions within the equipment. However, conventional grid-based and particle-based methods face various challenges when handling fluid flow in complex geometries. The immersed boundary method has emerged as a promising alternative to address these challenges. This method offers several advantages, including simplified mesh generation using orthogonal grids, ease of modifying geometries, and reduced computational costs. This report specifically focuses on the volume force-based immersed boundary method, presenting application examples including the simulation of Newtonian fluids, non-Newtonian fluids, porous media flow, and turbulent flow.

Introduction

Understanding the internal flow within the complex structures of chemical equipment is critical for its design and process optimization. In particular, a knowledge of the internal flow characteristics of chemical equipment is essential for achieving efficient reactions and enhancing product quality and yield. However, experimental investigation requires fabricating equipment for each condition, and it is difficult to observe three-dimensionally distributed quantities within the equipment. Thus, simulations are widely used to analyze the flow within equipment. Simulations require substantially lesser cost and time than experiments and enable detailed visualization of the flow behavior inside equipment. Conventional computational methods face challenges such as reduced accuracy and instability due to grid distortion, along with limited memory access. To address these issues, we developed programs based on the immersed boundary method to efficiently simulate internal flows. The immersed boundary method represents complex objects on a Cartesian grid by applying suitable external forces. The Cartesian grid offers advantages, including simpler mesh generation, easier geometry modifications, and reduced computational cost. This approach allows straightforward calculations of the flows in equipment with complex geometries, which is highly useful for design optimization and troubleshooting. This article introduces the immersed boundary method and provides computation examples.

Flow-simulation methods for complex geometries

(1) Previously developed methods

A variety of techniques have been developed and applied to simulate flows in equipment with complex geometries. For instance, grid-based methods divide a domain into a mesh for computation, including boundary-fitted grids aligned with boundaries and unstructured grids dividing the domain into polygonal cells. Particle methods have also been used, which involve computations using discrete points moving at the velocity of the fluid instead of dividing a domain using a mesh. These methods have the following known challenges. Boundary-fitted grids may require domain decomposition for complex geometries, and significant distortion in the grid can lead to instability. Furthermore, the governing equations become very complex, which increases the programming effort. Unstructured grids require substantial effort to generate, exhibit poor memory access and high computational costs because the points neighboring a cell are not stored adjacently, have poor convergence due to poorly shaped Poisson matrices, and complicate high-order solution methods. Particle methods suffer from poor memory access because discrete points move within the domain, and adjacency relationships change constantly. These methods also exhibit poor convergence due to poorly shaped Poisson matrices and have difficulty controlling the particle density. These drawbacks limit accuracy improvements, and thus, the immersed boundary method has gained attention in recent years.

The immersed boundary method uses a Cartesian grid to represent objects with complex geometries via external forces, which simplifies mesh generation. This method has all of the benefits of using a Cartesian grid, namely straightforward equation forms, efficient memory access, well-shaped Poisson matrices, and compatibility with high-order solution methods. The Cartesian grid also allows easy geometry modification, which shortens simulation lead times. Moreover, for complex geometries such as those of porous media, unstructured grids are an option; however, generating computer aided design (CAD) models from images of porous media is highly challenging. Even when possible, manual adjustments are generally required. Furthermore, when generating a mesh based on CAD, it is extremely difficult to divide the mesh while maintaining its quality, such as generating sharp boundaries, and the generated mesh must then be manually adjusted, which is time-consuming. The immersed boundary method enables the direct computation of the solid volume fraction in porous media from images, allowing simulations to proceed without concern for mesh quality and greatly improving the pre-computation efficiency. **Table 1** lists the results of a comparison of the flow simulation methods used for complex geometries. Based on this comparison, we develop programs that utilize the immersed boundary method.

(2) Types of immersed boundary methods

The immersed boundary method, which was developed by Peskin for simulating vascular flows, represents complex objects on a Cartesian grid by applying suitable external forces[1]. Immersed boundary methods are generally classified into continuous-forcing and discrete-forcing types[2]. In the continuous-forcing type, external forces are added to the governing equations prior to discretization to represent objects. By contrast, the discrete-forcing type adds external forces after discretization to represent objects. Various discrete-forcing approaches exist, including cut cells, ghost cells, and volume force-based methods. Consequently, many immersed boundary methods are available, and careful selection is required to determine the most appropriate method for a given application.

(3) Solid volume fraction type immersed boundary method

The solid volume fraction type immersed boundary method, which is a discrete forcing-type method developed by Kajishima, penalizes velocity according to the solid volume fraction of the object occupying each computational cell[3]. This method has broad applicability. Examples include solid–gas–liquid three-phase flows[4], oil–water separation via filters[5], mixing in gas–liquid two-phase flows[6], and heat transfer in solid–gas two-phase flows[7]. **Fig. 1** illustrates the concept of the solid volume fraction type immersed boundary method. In this method, complex boundaries are simulated by adding an external force to the Navier–Stokes equations. The magnitude of this external force is set to achieve a velocity consistent with the boundary conditions at the next time step. The calculation procedure is essentially identical to that of the fractional-step method[2], which is commonly used for velocity–pressure coupling in incompressible

Table 1 Comparison of numerical methods for flow in complex boundaries

Method	Mesh generation	Form of equation	Memory access	Poisson equation	High order scheme
Particle method	Not required	Unchanged	Slow	Difficult to solve	Slightly difficult
Boundary-fitted grid	Difficult	Complex	Fast	Normal	Applicable
Unstructured grid	Difficult	Unchanged	Slow	Difficult to solve	Difficult
Immersed boundary method	Easy	Unchanged	Fast	Easy to solve	Applicable

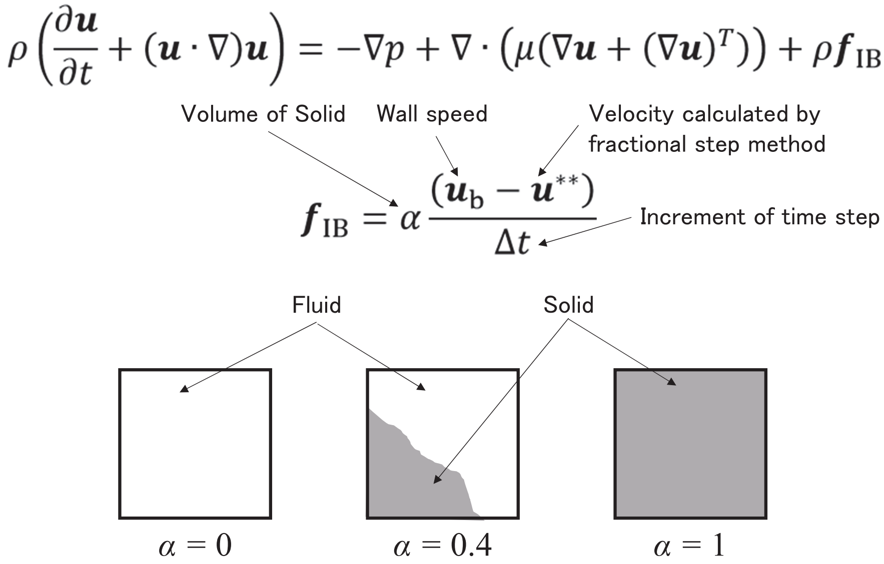

Fig. 1 Outline of volume of solid type immersed boundary method

flows, except for the addition of the external force at the final step. Furthermore, only the solid volume fraction, which can be determined geometrically, is required as a parameter. Thus, only the modification of a program for a Cartesian grid is enough for developing the program. Nevertheless, certain issues remain with the solid volume fraction type immersed boundary method. First, if the time step is not sufficiently small, inconsistencies such as pressure loss may occur, making preliminary checks of the time-step increment essential. Furthermore, as Ikeno *et al.*[8] noted, a naive application of discrete-forcing-type immersed boundary methods without internal iteration generally fails to satisfy both the solenoidal (incompressibility) condition and no-slip boundary condition simultaneously. Although this error is minor for laminar flows, care is required in turbulent flows. In flows with density differences, such as multiphase flows, these errors can adversely affect volume conservation.

In-house initiatives

(1) Computation example for Newtonian fluid

This section presents an example of how the immersed boundary method can be applied to a Newtonian fluid. A rectangular parallelepiped domain was used as the computational domain, with a horizontal circular pipe embedded within it. The fluid flowed in from the left and exited to the right. Periodic boundary conditions were applied at the inlet and outlet for simplicity. A pressure gradient was imposed on

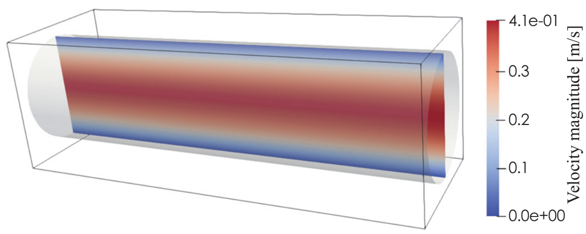

Fig. 2 Velocity magnitude of laminar flow in pipe

the initially stationary fluid, and computations were continued until a fully developed flow was achieved. **Fig. 2** displays the velocity magnitude within the circular pipe at a steady state. The results showed the development of the flow into a Poiseuille flow. This demonstrated that the immersed boundary method can accurately handle curved boundaries, such as circular pipes.

(2) Computation example for non-Newtonian fluid

Next, an example that combined the immersed boundary method with the numerical simulation of a non-Newtonian fluid is presented. The non-Newtonian fluid was shear-thinning, with the viscosity decreasing as the shear rate increased. The computational domain was a two-dimensional square containing cylinders representing a porous medium. The top and bottom surfaces were walls. The left surface was the inflow boundary, and the right surface was the outflow boundary. **Fig. 3** shows the velocity magnitude (contour) and direction (vector) of the non-Newtonian

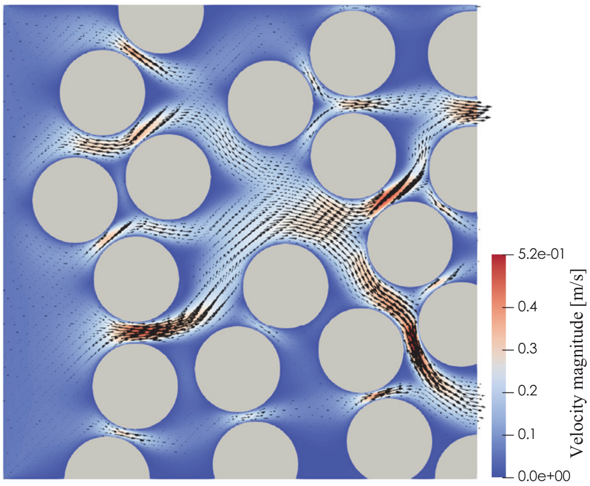

Fig. 3 Velocity magnitude and velocity vector of shear-thinning non-Newtonian fluid in porous media

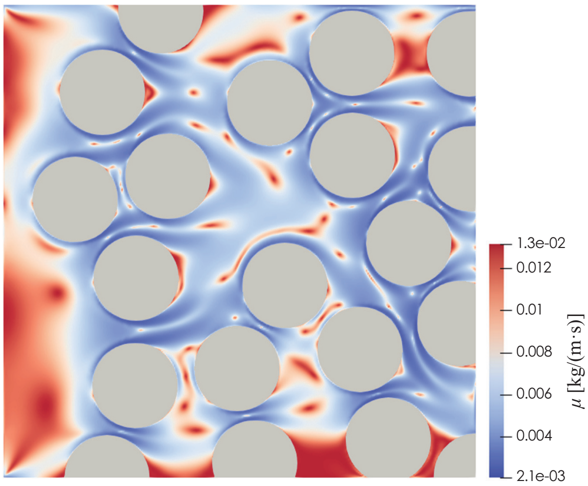

Fig. 4 Viscosity of shear-thinning non-Newtonian fluid in porous media

fluid flowing between the cylinders. **Fig. 4** illustrates the viscosity magnitude. **Fig. 3** confirms that the flow velocity increased in the area where the cylinders were closely spaced. Flow concentration regions could be observed within the porous medium. **Fig. 4** shows that the shear rate rose near the walls as a result of the no-slip condition, reducing the viscosity. The velocity gradients were smaller in the center of the channel, which produced low shear rates and a higher viscosity. This provided a detailed understanding of the viscosity field in a complex flow channel. Using conventional unstructured grids for these cylinder arrangements could lead to distorted meshes, reduced accuracy, instability, and longer computation times.

(3) Computation example for porous medium

Even in situations where unstructured or boundary-fitted grids are impractical, the immersed boundary method facilitates simulation. As an example, we present the results of calculations of the flow in a porous medium with a geometry that was more complex than that of a simple cylinder array. The domain was a two-dimensional rectangle containing the porous medium. The top and bottom surfaces are walls. The left surface was the inflow boundary, and the right surface was the outflow boundary. The solid volume fraction was determined directly from images and used to immerse the porous medium. **Fig. 5** shows the fluid velocity magnitude through the porous medium. The blue regions correspond to solid (0 m/s) areas, and the red regions indicate the fluid flow. **Fig. 5** highlights areas of flow concentration. The immersed boundary method enabled the computation of the pressure loss

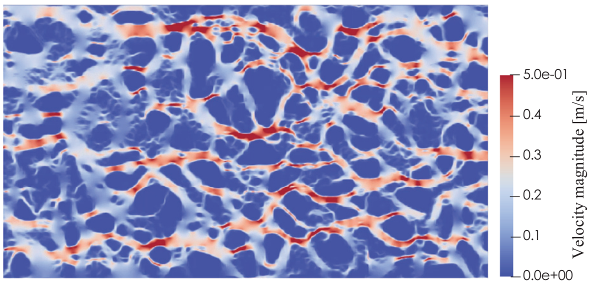

Fig. 5 Velocity magnitude in porous media

effects arising from flow variations due to the density of the porous medium. The direct computation of the solid volume fraction from images allowed efficient pre-computation preparation because the mesh-quality concerns were minimized. This technique is expected to aid in the future understanding of the flow between catalysts and support membrane-design applications.

(4) Computation example for turbulent flow

Finally, we investigated the results when the immersed boundary method was combined with a numerical simulation of turbulent flow. Turbulent flow is common in engineering, but capturing vortices accurately requires very fine grids. Methods with poor memory access are impractical for such simulations. The immersed boundary method is anticipated to be highly effective in this context. A rectangular parallelepiped domain was used, with a horizontal circular pipe immersed. The fluid inflow was from the left, and the outflow was to the right. Periodic boundary conditions were applied at the inlet and outlet, and a pressure gradient was imposed to simulate a transition from laminar to turbulent flow. **Fig. 6** presents the velocity

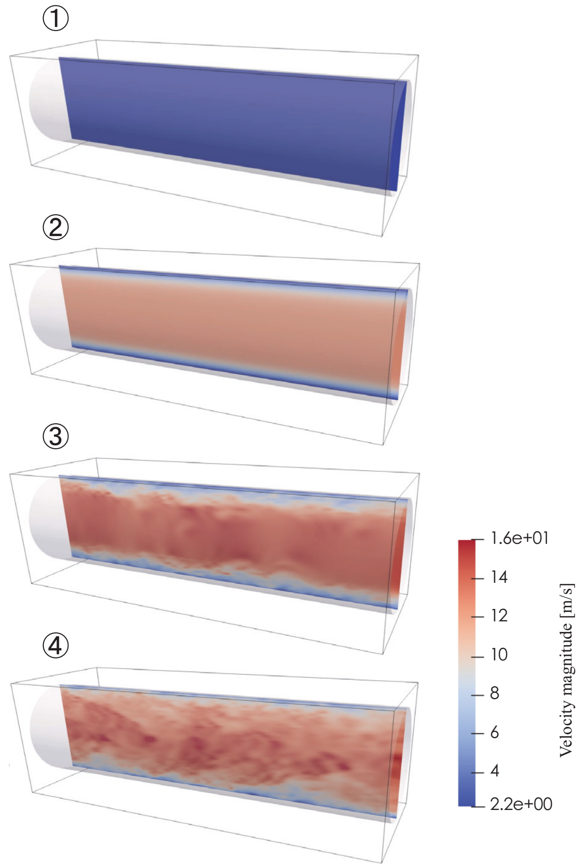

Fig. 6 Velocity magnitude of turbulent flow in pipe

magnitudes at several time points within the circular pipe. The results demonstrated a laminar-to-turbulent transition, with increasing velocity fluctuations and thinning boundary layers. Thus, combining the immersed boundary method with turbulent flow simulation allowed the accurate reproduction of the development of turbulence within circular pipes. Although periodic boundary conditions were applied here, sampling flow data can be used for the inlet, and convective outflow boundary conditions can be used for the outlet. The method could also be used to investigate flow effects due to instrumentation such as thermometers, as well as valve operability.

Conclusion

This paper introduced the immersed boundary method and computation examples. The focus was on the solid volume fraction type immersed boundary method. However, we are continually assessing suitable immersed boundary methods and developing simulations that incorporate turbulence, chemical reactions, and heat[9]. We are also considering coupling with multiphase flow, viscoelasticity, particles, and radiation[10]. Coupling the immersed boundary method with various physical models is nontrivial, and careful consideration is necessary. In the future, we aim to develop a multi-physics simulator based on this method for use in reactor/equipment design, process optimization, and other applications in order to accelerate our business activities.

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