Lattice Boltzmann Method development of PEMFC in mesoscopic scale

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Abstract: Proton exchange membrane fuel cell (PEMFC) mainly relied on the modeling analysis of the traditional numerical method. However, the scale of the research is bigger than porous medium layer of the particle that can’t meet the actual mechanism of the simulation. Hence, as a new mesoscopic numerical method, Lattice Boltzmann method (LBM) builds a model based on the microstructure and analyzes the dynamics, while the transfer state of the porous media layer of PEMFC can be more realistically described during its actual operation.

1. Introduction

As a new power generation technology, water and electric energy through the reaction of hydrogen and oxygen with the advantages of high energy conversion efficiency, low working temperature, low noise and no pollution through PEMFC generated. PEMFC has a great application prospect in automobiles and distributed energy sources [1].

Complexed research can be conducted with the mechanism of PEMFC, compared with the traditional method of CFD, smaller scale and complexed fluid flow of solid structure can be simulated by LBM. While, LBM has been applied to the research of PEMFC, such as personal relationship caused water to water simulation [1-3], capillary pressure simulation multi component mass transfer and electrochemical reaction [4-5], liquid water transmission [6].

2. Lattice Boltzmann method (LBM)

LBM is a mesoscopic computational fluid mechanics method based on the Molecular dynamics theory, microscopic scale and the macroscopic scale are connected by Boltzmann in it. LBM can completely simulate the N-S equation [8-9] at the macroscopic scale, and can deal with the complex boundary conditions and thermodynamic characteristics of multiphase flow more directly, and it is easy to conduct parallel calculation. In LBM, the motion of all particles is analyzed as a whole [10]. In the development of LBM, the establishment of discrete velocity model is the most important, in 1992, Qian discrete velocity model proposed by [11] is by far the most commonly used model, it is used in multiple dimensions and can be divided into different grids for analysis, as shown in fig. 1. Finally, the solution is carried out according to the direction of grid points, boundary conditions and equilibrium function.
LBM can be expressed as:

\[ f_k(x, y, t + \Delta t) = (1 - \omega)f_k(x, y, t) + \omega f^eq_k(x, y, t) \]  (1)

\( k \) is the component in fluid calculation, \( f_k \) is the distribution function calculated along the \( k \) direction, \( f^eq_k \) is the equilibrium distribution function, \( \Delta t \) is the time step, \( \omega \) is the relaxation frequency, and \( \omega = 1/\tau \), \( \tau \) is relaxation time.

LBM can be divided into two steps. The first step is to reconstruct the structure, and the second step is to solve the physical problem. Reasonable structural reconstruction can achieve ideal and practical simulation results. Structural models are classified according to dimensions, which are mainly divided into two-dimensional model and three-dimensional model. According to the reconstruction method, it is mainly divided into experimental scanning reconstruction and characteristic parameter reconstruction. The former mainly adopts three-dimensional imaging methods, such as X-ray tomographic imaging technology, to obtain relatively accurate structures and then convert them into digital models [12-25]. The latter is achieved by extracting specific information about on the sample and then creating a three-dimensional digital model with random microstructure [16-20].

3. Lattice Boltzmann method of fuel cell simulation

At present, fuel cell model mainly uses the macroscopic continuum model, and the mesoscopic scale simulation is mainly analyzed by macroscopic parameters [21-23]. Its model is greatly different from the actual structure, and it has certain limitations on the microscopic scale. LBM can reflect the physical structure more realistically, and the research mechanism is more consistent with the real dynamic behavior.

3.1. Single-phase and multi-component mass transfer simulations

The microstructure of porous media plays an important role in the transport of reactive materials. The macroscopic model simplifies the porous media layers such as GDL and CL into homogeneous and isotropic porous materials. However, due to the existence of micro-scale effects, characteristics of microstructure, interaction mechanism in the process of material transmission and other mechanisms are still unclear, the macroscopic model has certain limitations. In addition, it is of great significance to establish a single-phase multi component mass transfer model for the property research of PEMFC, due to the reaction materials in PEMFC mainly exist on the gaseous state. However, the presence of liquid water greatly affects the property improvement on PEMFC. Therefore, the establishment of multiphase and multi component mass transfer model is of great significance to the water management of PEMFC and the understanding of the evolution mechanism of liquid water.

3.2. Multi-phase and multi-component mass transfer simulation

Porous media contains multi component and multiphase states in operation, and LBM methods have been used to simulate two-phase flows of PEMFC [24-26]. Some scholars [12] proposed a three-dimensional two-phase lattice Boltzmann model based on the interaction potential to study the effects of pore structure and surface wettability in the catalyst layer (CL) and the gas diffusion layer (GDL) on the transport of liquid water and interface dynamics. Some scholars [13] also used LBM method to
model four different gas diffusion layers (GDL) and predict the liquid saturation of GDL. Some scholars [14] used LBM to numerically simulate the change of local saturation of PEMFC with or without microporous layer (MPL). Different from the single-phase and multi-component model, the multi-phase and multi-component model has to solve the problem of interface expression. The interface expression methods currently adopted by the mainstream of LBM multi-phase and multi-component model include Shan-chen model [15], Color model, Level set model, etc.

3.3. Simulation of phase transition process

In the phase transition simulation research, the research mainly focuses on the melting behavior at the scale of representative volume element (REV) [27-28], and some scholars [29] have also studied the phase transition at the pore scale. However, due to the changes in thermophysical properties before the phase transition and after it, the simulation results can hardly meet the actual mechanism. Compared with FVM and other methods, LBM can well explain the internal phenomena of porous structure. However, in complex structural problems, mass of computing resources are needed. Therefore, it is necessary to carry out the research on multi-scale coupling model.

3.4. Multi-scale coupling simulation

The multi-scale decomposition method decomposes the solving domain into several sub-domains, and then applies the corresponding optimal numerical method to simulate respectively [16-19]. There are two problems of multi-scale coupling. On the one hand, the source term is processed. In LBM, the source term is derived by formula and then reflected on the equilibrium distribution function, while Macroscopic numerical simulation method directly solves the source term discretely. On the other hand, the grid habit, in order to transmit information, needs to be redesigned in combination with two scale grids. In order to solve such problems, scholars [18] developed CFVLBM by derivation and upgrading the macro concentration to the concentration distribution function, and used it to simulate the fluid flow and mass transport in PEMFC. CFVLBM can effectively obtain the pore size information on GDL without the use of empirical relations and a large amount of computational resources.

4. Conclusion and Prospect

The continuum model cannot be related to the actual structural optimization due to the homogenization of the structure, while LBM can simulate the fluid phenomenon in mesoscopic view of the simplified dynamic model, and in addition, LBM can simulate the physical state of the fluid through the force between particles. When the problem is complicated, or the simulation accuracy improves, the computational resources need to be considered, as well as better and faster simulation results. In terms of specific research direction, the multi-phase and multi-component massed to transfer model of LBM gradually becomes the mainstream analysis method, while in the multi-phase model, the realization of interface recognition is the main problem. The phase transition not only exists on the cold starting process, but also affects the properties of PEMFC by the mutual transformation from liquid to gas. In the phase transition model, the determination of source term and thermophysical property is the main problem. Multi-scale models to tend to analyze the whole mass transfer process of PEMFC, in which the source termed derivation and grid coordination are the main problems to achieve the information transfer of multi-scale models.

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