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A COMPARISON BETWEEN LATTICE-BOLTZMANN AND FINITE-ELEMENT SIMULATIONS OF FLUID FLOW IN STATIC MIXER REACTORS*

D. KANDHAI[†,§], D. J.-E. VIDAL[‡,**], A. G. HOEKSTRA[†,¶], H. HOEFSLOOT[‡,††], P. IEDEMA[‡,‡‡], and P. M. A. SLOOT[†,‖]

[†]*University of Amsterdam*
Faculty for Mathematics, Computer Science, Physics, and Astronomy
Kruislaan 403, 1098 SJ Amsterdam, The Netherlands

[‡]*University of Amsterdam, Department of Chemical Engineering*
Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands

[§]*E-mail: kandhai@wins.uva.nl*
[¶]*E-mail: alfons@wins.uva.nl*
[‖]*E-mail: peterslo@wins.uva.nl*
http://www.wins.uva.nl/pscs
[**]*E-mail: vidal@chemeng.chem.uva.nl*
[††]*E-mail: huubh@chemeng.chem.uva.nl*
[‡‡]*E-mail: piet@chemeng.chem.uva.nl*
http://ctuww.chem.uva.nl

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We present a comparison between the finite-element and the lattice-Boltzmann method for simulating fluid flow in a SMRX static mixer reactor. The SMRX static mixer is a piece of equipment with excellent mixing performance and it is used in highly efficient chemical reactors for viscous systems like polymers. The complex geometry of this mixer makes such 3D simulations nontrivial. An excellent agreement between the results of the two simulation methods and experimental data was found.

Keywords: Static Mixer Reactor; Lattice-Boltzmann; Finite-Element Method.

1. Introduction

The lattice-Boltzmann method[1–3] is a new approach in computational fluid dynamics. It originated from the lattice-gas model[4] and has a microscopic character, as opposed to the conventional approach based on a numerical solution of the Navier–Stokes equation.[5] The key idea behind this method is to model fluid flow by distributions of particles moving on a regular lattice. At each time step the particles propagate to a neighboring lattice point followed by local collisions in which their velocities are redistributed.

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This simulation model has proven to be successful in modeling and simulation of complex fluid dynamical problems for which the conventional macroscopic approach may be difficult to apply. These simulations include solid-fluid suspensions,[6,7] multiphase flows[8] and the effect of convection-diffusion on growth processes.[9] Also, flow in complex geometries, e.g., fluid flow in porous media, has been successfully simulated with this method.[10] Another important advantage of the lattice-Boltzmann method is the inherent spatial locality of the updating rules. This property makes it ideal for parallel processing.[11]

Although this approach has proven to be very useful for simulating complex fluid flows, examples of its use in realistic engineering applications are still limited. The main reason for this, is the fact that the method has mostly been used for studying academic problems. Moreover, only a few benchmark studies (see e.g., Refs. 13 and 14) which focus on a comparison with state of the art traditional methods and experimental data from both a numerical and computational point of view, has been reported.

In this contribution we briefly present a comparison between the lattice-Boltzmann, the Finite-Element method and experimental data. In a companion communication, a detailed comparison between both methods will be presented.[12] We intend to show that the lattice-Boltzmann method is a good alternative to the traditional macroscopic momentum balance methods for computing fluid flows in complex geometries. As a benchmark problem we take fluid flow in a 3D static mixer reactor,[15] a technology introduced 15–20 years ago, which has gained more and more in popularity within the chemical industry over recent years. A SMRX

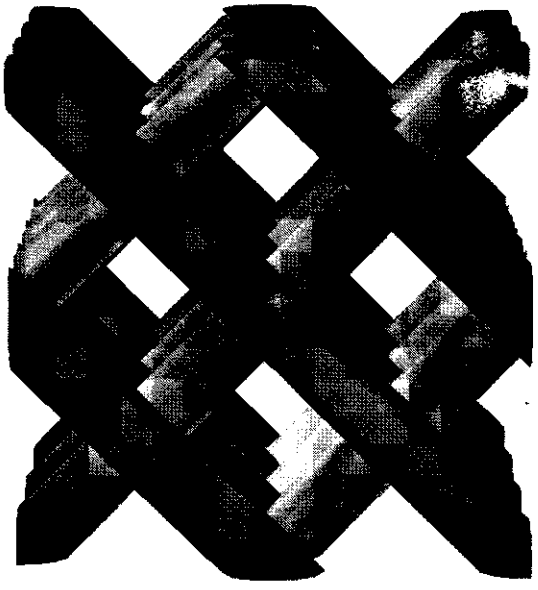

Fig. 1. A SMRX static mixer element.

reactor is a plug-flow type reactor filled with a series of SMRX static mixer elements (see Fig. 1) turned at 90 degrees with respect to each other. The mixer element consists of specially designed stationary obstacles in order to promote mixing of fluid streams flowing through it. Its mixing mechanism relies on splitting, stretching, reordering and recombination of the incoming fluid streams. In this communication we focus on only one SMRX element for obvious reasons of simplicity. Due to usually rather complex flows and geometries, only few 3D numerical simulations of flow through static mixers were performed in the past.[16]

In Sec. 2 we discuss the basic idea of simulating fluid flow by the Finite-Element and the lattice-Boltzmann methods. In Sec. 3 we show the numerical results. And in the last section the conclusions are presented.

2. Two Ways of Modeling Hydrodynamics

In this section we present the basic fundamentals of the finite-element (FEM) and the lattice-Boltzmann (LBM) methods. The aim is to underline the conceptual differences between the two methods.

The FEM is based on a numerical solution of a macroscopic description of fluid flow, which in the case of an incompressible fluid in a given geometry Ω can be described by the classical Navier–Stokes equations[5]

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) + \nabla\cdot\sigma + \nabla p = \mathbf{f}, \tag{1}$$

$$\nabla\cdot\mathbf{v} = 0, \tag{2}$$

where ρ is the fluid density, $\mathbf{v}$ is the velocity, p is the pressure and $\mathbf{f}$ is a body force, e.g., the gravity force. The stress tensor σ is a function of the rate-of-strain tensor $\dot{\gamma} = \frac{1}{2}(\nabla\mathbf{v} + (\nabla\mathbf{v})^T)$, through a rheological model:

$$\sigma = -2\eta\dot{\gamma}, \tag{3}$$

where, depending on the rheological model chosen, the fluid viscosity η could be a function of $|\dot{\gamma}|$ (non-Newtonian models) or simply equals to the Newtonian viscosity μ.

The finite-element method for solving fluid flow dynamics makes use of variational calculus which allows the transformation of a set of partial differential equations (in our case, the Navier–Stokes equations) into a system of linear algebraic equations.[17] This can be solved using a simple LU decomposition or by means of iterative algorithms.

The lattice-Boltzmann method on the other hand is a mesoscopic approach where the macroscopic dynamics is approximated by interactions between fictitious particles on a regular lattice. The main idea here is that fluid flow is mainly determined by the *collective* behavior of many molecules and not really by the detailed molecular interactions. Basically the time-evolution of the lattice-Boltzmann algorithm consists of the following two phases:

1. *Propagation.* In this phase particles move along lattice bonds from one lattice node to one of its neighbors.
2. *Collision.* Particles on the same lattice redistribute their momenta locally, subject to mass and momentum conservation.

In this article we use the so-called lattice-BGK (Bhatnagar–Gross–Krook) model, where the collision operator is based on a single-time relaxation to the local equilibrium distribution,[2,13]

$$f_i(\mathbf{r}+\mathbf{c}_i, t+1) = f_i(\mathbf{r},t) + \frac{1}{\tau}\Big(f_i^{(0)}(\mathbf{r},t) - f_i(\mathbf{r},t)\Big), \tag{4}$$

where $\mathbf{c}_i$ is the ith link, $f_i(\mathbf{r},t)$ is the density of particles moving in the $\mathbf{c}_i$-direction, τ is the BGK relaxation parameter, and $f_i^0(\mathbf{r},t)$ is the equilibrium distribution function towards which the particle populations are relaxed.[2,13]

It is obvious that FEM and LBM are two very different numerical approaches. FEM is based on approximations of flow equations that are governed by basic physical conservation laws on the *macroscopic* scale, whereas LBM is based on evolution rules which obey the same conservation laws on a *mesoscopic* scale. In LBM the physical evolution rules are discrete while in FEM methods the discretization is performed on the level of the macroscopic flow equations.

3. Numerical Results

In this section we present the results, namely the pressure along the SMRX mixer using both methods. The experimental results of van Dijck *et al.*[19] for the pressure drop at different flow rates are used to validate both numerical methods. Before going into details we first briefly discuss some practical issues of both simulation methods.

Concerning the FEM simulations, the first step was to generate a satisfactory mesh of the SMRX geometry. Using a commercial mesh generator (SDRC's I-DEAS package) we succeeded in creating two adequate meshes made of roughly 35 000 tetrahedral elements. In our meshes, we used two types of tetrahedral elements, namely the $P_1^+ - P_0$ elements (called linear elements) and the $P_2^+ - P_1$ elements (called quadratic elements).[18] The flow simulations were performed on one RISC6000 77 MHz node of an IBM 9076 SP2 with 512 MB of nodal memory using POLY3D^{TM} from Rheotek. The memory space usage was 129 MB and 480 MB respectively for $P_1^+ - P_0$ and $P_2^+ - P_1$ meshes. The computational time was 40 CPU min and 190 CPU min respectively.

In LBM the geometry is represented on a uniform Cartesian grid. Each grid point is marked as a solid point when it belongs to an obstacle and otherwise it is marked as a fluid point. To obtain a satisfactory discretization of the SMRX element we have used lattices of dimension $112 \times 56 \times 56$ and $224 \times 112 \times 112$ grid points, based on a tube radius discretization of 4 and 8 grid points respectively. The flow simulations were performed on a 32-node Parsytec CC parallel machine

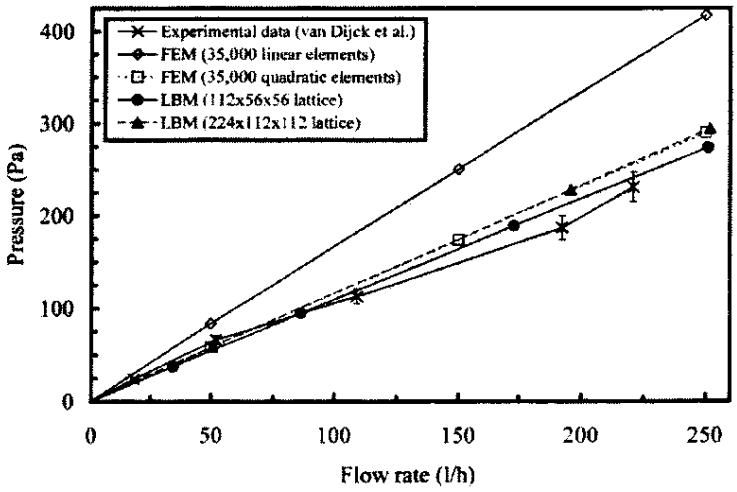

Fig. 2. Pressure drop versus flow rate.

with 128 MB memory per node (133 MHz PowerPC 604). The total memory space usage was 50 MB and 400 MB for the $112 \times 56 \times 56$ and $224 \times 112 \times 112$ lattice respectively. The computational time on one node of the parallel machine was 110 CPU min and 3300 CPU min (estimated, because this simulation could not be executed on a single node of the machine due to memory constraints) respectively. However, the real runs were performed on 16 nodes of the parallel machine and then the computation time was 10 CPU min (parallel efficiency[11] of 0.7) and 210 CPU min (parallel efficiency estimated to be close to 1) for the two grid resolutions.

The pressure drop as a function of the flow rate is shown in Fig. 2. Here we have included the results obtained by the two methods on the different grids and meshes. We see that for FEM there is a big discrepancy between the $P_1^+ - P_0$ and the $P_2^+ - P_1$ meshes for all flow rates. The LBM results on the two grids are quite close to each other. We clearly see that indeed the FEM and the LBM solutions converge to each other as the grid or mesh-element type is refined. These results are also good in agreement with the experimental data of van Dijck *et al.*[19] The systematic error in the experimental data is approximately 7% for the pressure measurements. For low flow rates the simulations are in the estimated error range of the experimental data. For higher flow rates the simulations over estimate the pressure drop. The maximum difference between simulations and experiment is around 15%. These differences may be caused by experimental uncertainties in the calibration of the flow rate and in viscosity measurements. Notice that in both simulations, we have assumed that the fluid is Newtonian, whereas from experimental measurements it was evident that the fluid is not purely Newtonian.[19] Furthermore, more detailed experimental measurements (at least more data points) are required in order to judge the actual cause of the slight disagreement between simulations and experiments.

4. Conclusions

Our results indicate that the level of agreement between both simulation methods is astonishingly high. Moreover, the simulated data fits well with the experimental values.

In the case tested, the LBM uses roughly 10 times less memory than the FEM to reach a similar accuracy, since the solution given by the LBM coarse grid already reaches a satisfactory precision. Although the simulations were not executed on the same computer, it appears also that the LBM coarse grid simulation requires roughly the same computational time (on a sequential machine) compared to the FEM fine mesh simulation. However, the computational time required by the LBM fine grid simulation shows a drastic increase compared to the coarse grid simulation.

In a companion communication we will present this study in much more detail, including a comparison of the local velocity and pressure profiles, fluid flow in more complicated reactors and a methodological comparison between the two methods.[12]

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