TASK QUARTERLY 9 No 4, 449–459

MIXING IN A STIRRED VESSEL. A PARALLEL IMPLEMENTATION WITH LATTICE BOLTZMANN COLOURED PARTICLES MODEL

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(Received 10 July 2005; revised manuscript received 2 September 2005)

Abstract: The main purpose of this paper is to present a new method for the study of single fluid mixing in a stirred vessel. The simulation has been realized with a parallel implementation of the Lattice Boltzmann coloured particles model. The mixing phenomenon is compared with the one derived with a Lagrangian approach.

Keywords: lattice Boltzmann, parallel algorithm

1. Introduction

The main purpose of Computational Fluid Dynamics (CFD) is to investigate the behavior of fluid flow under various conditions. The motion of an isothermal and incompressible fluid is described by the continuity equation and the Navier-Stokes equation. The complexity of this differential system is due to the non-linear terms.

Lattice Boltzmann Models (LBMs) are a relatively recent technique to simulate fluid motion (see [1–6]). The basic idea of LBMs is to model the macroscopic behavior of a fluid by implementing microscopic interactions between its particles. This approach leads to an easy parallelizable procedure capable of simulating flow in complex geometries.

LBMs were initially derived from Lattice Gas Cellular Automata but this approach involved some problems such as statistical noise, low Reynolds number and increased complexity of the collision operator when one tries to increase the number of dimensions from two to three. In 1988, McNamara and Zanetti, [7], proposed the first Lattice Boltzmann equation in order to overcome the statistical noise problem. From this moment the evolution accelerated until it produced the simplest Lattice Boltzmann Equation, the so-called Lattice-Bhatnagar-Gross-Krook equation (LBGK), [8], based on single relaxation time approximation. It has also been shown that the Lattice Boltzmann Equation can be viewed as a discretization of the continuum Boltzmann BGK equation [9].

In LBMs space is discretized by a regular lattice (square or hexagonal for two-dimensional domains and cubic for three dimensional domains) and a distribution function of flow density is defined at each discrete lattice point. The model evolution consists of two alternating steps: relaxation of the distribution function to local equilibrium in each node (collision) and propagation of the fluid to the nearest neighbours of the lattice (propagation).

The aim of this work has been to study the mixing of a fluid in a stirred vessel with an easy and parallelizable algorithm. This problem was already developed in [10] where the velocity field was modelled by LBM D3Q19 and the particles' trajectories were restored with a Lagrangian approach. The main disadvantages of this technique are a strong load imbalance when each processor knows only its own velocity field with fine grids and the massive memory use when the whole velocity field is stored in each processor (see [11]).

We have used the Lattice Boltzmann Coloured Particles Model (LBCPM) similar to that proposed by E. G. Flekkøy, [12], for miscible binary fluids. To observe mixing we mark some particles introducing a colour distribution function. Its evolution is based on a Lattice Boltzmann scheme with an appropriate equilibrium distribution, [13]. We will show that the LBCPM offers a qualitative and quantitative description of the mixed fluid very similar to that obtained in [10] with the coloured particles tracking method (CPTM). Furthermore, this method allows us to take advantage of all the computational merits of LBMs. Comparability of the models has been the only reason for the particular choice of the domain geometry and the physical constants.

2. The Boltzmann model for miscible fluids

Let us consider a viscous, incompressible and isothermal fluid that completely fills a mixer with four rotating blades. The motion is described by the continuity equation:

$$\boldsymbol{\nabla}\cdot\boldsymbol{u}=0, \tag{1}$$

and by the dimensionless Navier-Stokes equation:

$$\frac{\partial\boldsymbol{u}}{\partial t}+(\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u}=-\boldsymbol{\nabla}P+\frac{1}{\mathrm{Re}}\nabla^2\boldsymbol{u}, \tag{2}$$

where $t\in[0,T]$, $\boldsymbol{x}=(x_1,x_2,x_3)\in\Omega\subset\mathbb{R}^3$, and the dimensionless vector function $\boldsymbol{u}(\boldsymbol{x},t)=(u_1,u_2,u_3)$ represents the fluid velocity.

With fixed length, l_b, of each blade and velocity, ω_b, of the impeller, the kind of the fluid is represented by the Reynolds number:

$$\mathrm{Re}=\frac{4l_b^2\omega_b}{\nu}\,, \tag{3}$$

where $\nu=\frac{\mu}{\rho}$ is the kinematic viscosity of the fluid, *i.e.* the ratio between its absolute viscosity, μ, and its density, ρ.

To compare the LBCPM and the CPTM, we have chosen the domain already presented in [10], it has the shape of a frustum of a right circular cone:

$$T_C=\left\{(x_1,x_2,x_3)\in\mathbb{R}^3\,:\,0<x_3<z_s,\ (x_1^2+x_2^2)<\left(\frac{r_s-r_i}{z_s}x_3+r_i\right)^2\right\}, \tag{4}$$

where r_i, r_s are the radii of the lower and the upper base and z_s is its height. The impeller is modelled by a right, circular cylinder C:

$$C = \left\{(x_1, x_2, x_3) \in \mathbb{R}^3 : z_m \le x_3 \le z_M,\ (x_1^2 + x_2^2) \le (r_C)^2\right\}, \tag{5}$$

where r_C is its radius and $z_M - z_m$ is its height. These parameters must verify the following relationships: $0 < r_i, r_s$, $0 < z_m < z_M < z_s$, and $0 < r_C < \left(\dfrac{r_s - r_i}{z_s} z_m + r_i\right)$.

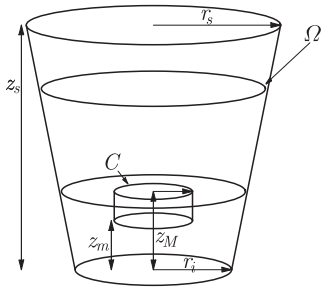

Figure 1. Position of the impeller inside the vessel with $r_i = 4.5 \cdot 10^{-2}$ m, $r_s = 6.6 \cdot 10^{-2}$ m, $r_c = 2.75 \cdot 10^{-2}$ m, $z_m = 2.4 \cdot 10^{-2}$ m, $z_M = 3.3 \cdot 10^{-2}$ m, $z_s = 1.68 \cdot 10^{-1}$ m

Four blades determine the shape of the impeller (see Figure 1). Initially we put them along directions $\theta_i = \frac{i\pi}{2}$ with $i = 0, \ldots, 3$, at the height of $z_0 = \frac{1}{2}(z_m + z_M)$. Our model has a maximum angular speed of $\omega_b = 4\pi$, so that the blades' position is $\theta(t) = \theta_i + \omega_b t$, $t > 0$. We model them so that the blades along the θ_0 and θ_2 directions produce upward vertical speed while those at θ_1 and θ_3 produce downward vertical speed (see [14]).

The domain is:

$$\Omega = T_C \setminus C, \tag{6}$$

and its boundary is $\partial\Omega = \Gamma_0 \cup \Gamma_1 = \Gamma$, where

$$\Gamma_0 = \partial T_C, \Gamma_1 = \partial C. \tag{7}$$

The Lattice Boltzmann Model is applied to simulate the dimensioned velocity field of an incompressible fluid when mixed by the impeller. The chosen model is D3Q19, a multi-speed model with a cubic lattice (Figure 2).

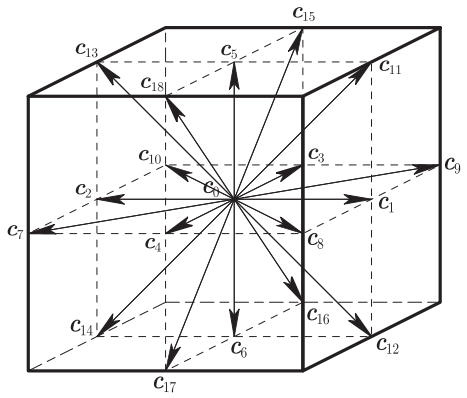

Figure 2. Cubic lattice with 19 velocity directions

We consider the frustum of the right circular cone T_C enclosed in a parallelogram with the following discrete lattice:

$$G_\sigma = \big\{(x_1^m, x_2^n, x_3^k) \in \mathbb{R}^3 : x_1^m = -r_s + m\sigma,\ x_2^n = -r_s + n\sigma,\ x_3^k = k\sigma,\ m,\ n = 0,\ldots,n_x,\ k = 0,\ldots,n_z\big\}, \tag{8}$$

where σ is the minimal distance between two grid points. We set $n_x = 2r_s/\sigma$ and $n_z = z_s/\sigma$. Points $\boldsymbol{x} \in T_C$, called active points, define the domain where the simulation takes place, whereas the boundary condition of the vessel is imposed at points $\boldsymbol{x} \in \partial T_C$. The remaining points of the lattice are defined as inactive.

In the stirred vessel, T_C, we put a single, isothermal and incompressible fluid whose density, $\rho(\boldsymbol{x},t)$, is represented by the mass distribution functions F_i as follows:

$$\rho(\boldsymbol{x},t) = \sum_{i=0}^{18} F_i(\boldsymbol{x},t). \tag{9}$$

$F_i(\boldsymbol{x},t)$ represents the mass fraction of the fluid moving with velocity $\boldsymbol{c}_i$ from the node in position $\boldsymbol{x}$ at time t. The set of velocities $\boldsymbol{c}_i$, $i = 0,\ldots,18$, is defined by the D3Q19 model. At the same time we consider the total momentum density of the fluid:

$$\boldsymbol{j}(\boldsymbol{x},t) = \sum_{i=0}^{18} F_i(\boldsymbol{x},t)\boldsymbol{c}_i = \rho\boldsymbol{u}. \tag{10}$$

Initially, the fluid fills the stirred vessel completely and remains at rest:

$$\begin{aligned} &\rho(\boldsymbol{x},0) = \rho_0,\ \boldsymbol{x} \in T_C, \\ &\boldsymbol{j}(\boldsymbol{x},0) = 0,\ \boldsymbol{x} \in T_C. \end{aligned} \tag{11}$$

To visualize mixing we mark a small part of the fluid by defining a colour function:

$$\delta(\boldsymbol{x},t) = \sum_{i=0}^{18} C_i(\boldsymbol{x},t). \tag{12}$$

At time $t = 0$ we choose to colour a fraction of the fluid $S \subset T_C$:

$$\begin{aligned} &\delta(\boldsymbol{x},0) = \delta_0,\ \boldsymbol{x} \in S, \\ &\delta(\boldsymbol{x},0) = 0,\ \boldsymbol{x} \in T_C \setminus S. \end{aligned} \tag{13}$$

At each node, the density and colour of the fluid are shared between the lattice vectors according to the equilibrium weights. In the D3Q19 model we have:

$$\begin{aligned} W_i &= \frac{1}{3} \quad i = 0, \\ W_i &= \frac{1}{18} \quad i = 1,\ldots,6, \\ W_i &= \frac{1}{36} \quad i = 7,8,\ldots,18. \end{aligned} \tag{14}$$

Then, $F_i(\boldsymbol{x},0) = \rho_0 W_i$ and $C_i(\boldsymbol{x},0) = \delta(\boldsymbol{x},0)W_i$, $\boldsymbol{x} \in T_C$.

The dynamics of the fluid is performed by the Boltzmann kinetic equation in the BGK approximation:

$$F_i^\star(\boldsymbol{x},t+1) = F_i(\boldsymbol{x},t) + \omega(F_i^{(eq)}(\boldsymbol{x},t) - F_i(\boldsymbol{x},t),) \tag{15}$$

and for the colour:

$$C_i^{\star}(\boldsymbol{x},t+1) = C_i(\boldsymbol{x},t) + \lambda_D(C_i^{(eq)}(\boldsymbol{x},t) - C_i(\boldsymbol{x},t)), \tag{16}$$

where $F_i^{(eq)}(\boldsymbol{x},t)$ and $C_i^{(eq)}(\boldsymbol{x},t)$ are the equilibrium distributions:

$$F_i^{(eq)}(\boldsymbol{x},t) = W_i\,\rho\left\{1+3\,\boldsymbol{c}_i\cdot\boldsymbol{u}+\frac{9}{2}(\boldsymbol{c}_i\cdot\boldsymbol{u})^2-\frac{3}{2}\,\boldsymbol{u}^2\right\}, \tag{17}$$

$$C_i^{(eq)}(\boldsymbol{x},t) = \frac{\delta(\boldsymbol{x},t)F_i(\boldsymbol{x},t)}{\rho(\boldsymbol{x},t)}\,. \tag{18}$$

The velocity, $\boldsymbol{u}$, of the fluid is given as follows:

$$\begin{aligned} \boldsymbol{u} = \frac{\boldsymbol{j}}{\rho} = \frac{\sum_{i=0}^{18}\boldsymbol{c}_i F_i}{\sum_{i=0}^{18} F_i} \qquad & \boldsymbol{x}\in\Omega\,, \\ \boldsymbol{u} = \boldsymbol{v} \qquad & \boldsymbol{x}\in C\,, \end{aligned} \tag{19}$$

where $\boldsymbol{v}(\boldsymbol{x},t)$ is the known velocity of the impeller blades. The first relaxation parameter, ω, defines the kinematic viscosity:

$$\nu = \Delta t c_s^2\left(\frac{1}{\omega}-\frac{1}{2}\right), \tag{20}$$

where $c_s = \sigma/(\sqrt{3}\Delta t)$ is the sound speed in the D3Q19 model and Δt is the time step. The ω value is deduced from the Reynolds number

$$\mathrm{Re} = \frac{4l_b^2\omega_b}{\nu} = \frac{4l_b^2\omega_b}{c_s^2\Delta t\left(\frac{1}{\omega}-\frac{1}{2}\right)} \quad\Rightarrow\quad \omega = \frac{1}{\frac{1}{2}+\frac{4l_b^2\omega_b}{c_s^2\Delta t\mathrm{Re}}}\,. \tag{21}$$

In the next step, we propagate the density and colour distribution functions, F_i and C_i, respectively, to the nearest neighbour along the i direction:

$$\begin{aligned} F_i(\boldsymbol{x}+\boldsymbol{c}_i,t+1) &= F_i^{\star}(\boldsymbol{x},t+1) \quad \boldsymbol{x}\in T_C\cap G_\sigma\,, \\ C_i(\boldsymbol{x}+\boldsymbol{c}_i,t+1) &= C_i^{\star}(\boldsymbol{x},t+1) \quad \boldsymbol{x}\in T_C\cap G_\sigma\,. \end{aligned} \tag{22}$$

We apply no-slip conditions on the boundary Γ_0 as in [10].

As shown in [13], the colour function, $\delta(\boldsymbol{x},t)$, with the chosen equilibrium distributions, Equation (18), satisfies the following equation:

$$\partial_t\delta + \boldsymbol{u}\cdot\boldsymbol{\nabla}\delta = \frac{\delta}{\rho}\left(\frac{1}{\lambda_D}-\frac{1}{2}\right)\partial_{x_a}\partial_{x_b}P_{ab}\,, \tag{23}$$

where summation over a and b is assumed and P_{ab} is the moment flux tensor:

$$P_{ab}(\boldsymbol{x},t) = \sum_i c_{ia}\,c_{ib}\,F_i(\boldsymbol{x},t) \qquad a,b=1,2,3. \tag{24}$$

It follows from Equation (23) that, if the value of the relaxation parameter λ_D is chosen as close as possible to two, the motion of coloured particles describes the fluid particles' trajectories very well.

3. Parallel implementation

In the last section we have established that fluid mixing can be modelled by the evolution of the colour function, $\delta(\boldsymbol{x},t)$. The full locality operation in Equations

(15), (16) and (22) allows an easy parallel implementation by applying the classical *domain decomposition* technique.

We divide the discrete domain along the Z axis into spatially contiguous blocks. The number of blocks equals the number of processors available in the cluster. The balance of the computational work between machines is realized by a bisection algorithm. Let us recall that grid points $\boldsymbol{x} \in G_\sigma$ are divided into active and inactive points, with negligible CPU time for the latter. Consequently, we split the lattice into parts containing the same number of active points. Let us suppose that our cluster has n, $n>1$, processors. We call h_i, $i=0,\ldots,n-1$, the height of frustum of the right circular cone memorized in processor i: we should find an array $\boldsymbol{h}=[h_0,\ldots,h_{n-1}]$ such that:

$$V(h_i)=V(h_j) \quad i,j=0,\ldots,n-1, \tag{25}$$

where $V(h_i)$ is the volume of the frustum stored in processor i:

$$V(h_i)=\frac{1}{3}\pi h_i(r_m^2+r_M^2+r_m r_M), \tag{26}$$

$r_m=r_m(h_i)$ and $r_M=r_M(h_i)$ being the smallest and the greatest radius of the subdomain.

Let $n=2^p$, $p\in\mathbb{N}$. First, we divide the volume of the whole frustum, T_C, by two along the Z axis, so that the two contiguous subdomains have the same number of active points. Then, the volume of each subdomain is further divided by two. We repeat this division p times until we obtain 2^p parts of the same volume. Finally, we store the points of the parallelepiped $H_0=\{\boldsymbol{x}\in G_\sigma : 0\le x_3\le h_0\}$ in the 0 processor, the points of $H_1=\{\boldsymbol{x}\in G_\sigma : h_0\le x_3\le h_1\}$ in the 1 processor, and so on. In this way the bottom of the vessel is placed in the master processor and the top – in the last processor of the cluster.

We define a border site as a node with at least one of its neighbours on the contiguous processor. Regular sites are nodes with own neighbours known by the same processor. In our problem, border sites are only situated in the first and the last levels stored in each processor. In the parallel implementation we can complete the streaming in the border sites only through data exchange between adjacent blocks. In each processor, the data of the higher sites are sent to the next client; similarly the lower sites pass information to the former client.

According to [14] and [10], the dimensions of our domain Ω are $r_i=0.045\text{m}$, $r_s=0.066\text{m}$, $z_s=0.168\text{m}$. The impeller occupies the right circular cylinder C with $r_C=0.0275\text{m}$, $z_m=0.024\text{m}$, $z_M=0.033\text{m}$. The blades' length is $l_b=r_C$. A parallelepiped encloses the Ω domain: its base is $r_s\times r_s$ and its height equals z_s. We have considered two discrete grids G_σ on the parallelepiped. One has a step of $\sigma=3.0\cdot10^{-3}\text{m}$; the obtained points are $n_x=45$ along the X and Y axes and $n_z=57$ along the Z axis. In the other grid the step is halved, $\sigma=1.5\cdot10^{-3}\text{m}$, and then $n_x=89$ along the X and Y axes and $n_z=112$ along the Z axis. In the first case we put $\Delta t=10^{-3}\text{s}$ and, if the simulations is based on the grid with $\sigma=1.5\cdot10^{-3}\text{m}$, the time step is halved.

We consider a fluid with a relatively low Reynolds number: $\text{Re}=250$. The relaxation parameter, ω, is univocally determined by Equation (21). We chose the

diffusion parameter to be $\lambda_D = 1.99$, the highest value that keeps the numerical stability of this single relaxation time model.

We assumed $\rho_0 = 0.1$ as the initial fluid density and concentrated all the coloured particles in the S region of the vessel, according to Equations (11) and (13), setting $\delta_0 = \rho_0$. For a qualitative study of the mixing as in [10], we chose (see Figure 3):

$$S = \{\boldsymbol{x} \in T_C : z_0 - 0.015\,\mathrm{m} \le x_3 \le z_0 + 0.015\,\mathrm{m},\ 0 \le x_1, x_2 \le r_i\}. \tag{27}$$

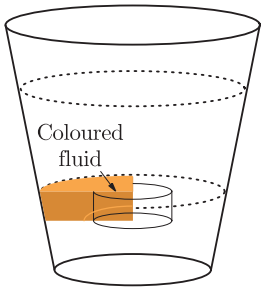

Figure 3. Initial position of the coloured particles

The simulations were performed on a cluster made by Xeon at 3.2 GHz with Debian as the operating system. They were connected via an Ethernet network at 1 Gbit/sec. Considering the SPMD paradigm, data exchanges were carried out by a MPICH library. The serial version of the model was run on a Xeon at 3.2 GHz. The CPU took 479 seconds for each second of the simulation on the coarse grid (1000 iterations) and 6400 seconds for the fine grid (2000 iterations).

We tested the parallel program on clusters with 2, 4 and 8 processors in order to evaluate the speedup, S_u, and efficiency, E_f. The results are shown in Table 1.

Table 1. Speedup and efficiency

	2 processors		4 processors		8 processors	
	S_u	E_f	S_u	E_f	S_u	E_f
$\sigma = 0.03\,\mathrm{m}$	1.90	95%	3.22	80.5%	5.28	66%
$\sigma = 0.015\,\mathrm{m}$	1.91	96%	3.44	86%	6.03	75%

4. Results

To check our simulation and measure the mixing in the model we imagine the T_C domain to be divided into layers L_k:

$$L_k = \left\{\boldsymbol{x} \in T_C \left(k - \frac{1}{2}\right) d_2 \le z \le \left(k + \frac{3}{2}\right) d_2\right\}, \quad k = 1, \ldots, 54, \tag{28}$$

where $d_2 = 3.0 \cdot 10^{-3}\,\mathrm{m}$. By analogy with the definition of the diffusion index given in [10], we chose to colour all lattice points located in region S_j of the vessel:

$$S_j = \{(x_1, x_2, x_3) \in T_C : b_j \le x_3 \le u_j,\ 0 \le x_1, x_2 \le r_i\}, \tag{29}$$

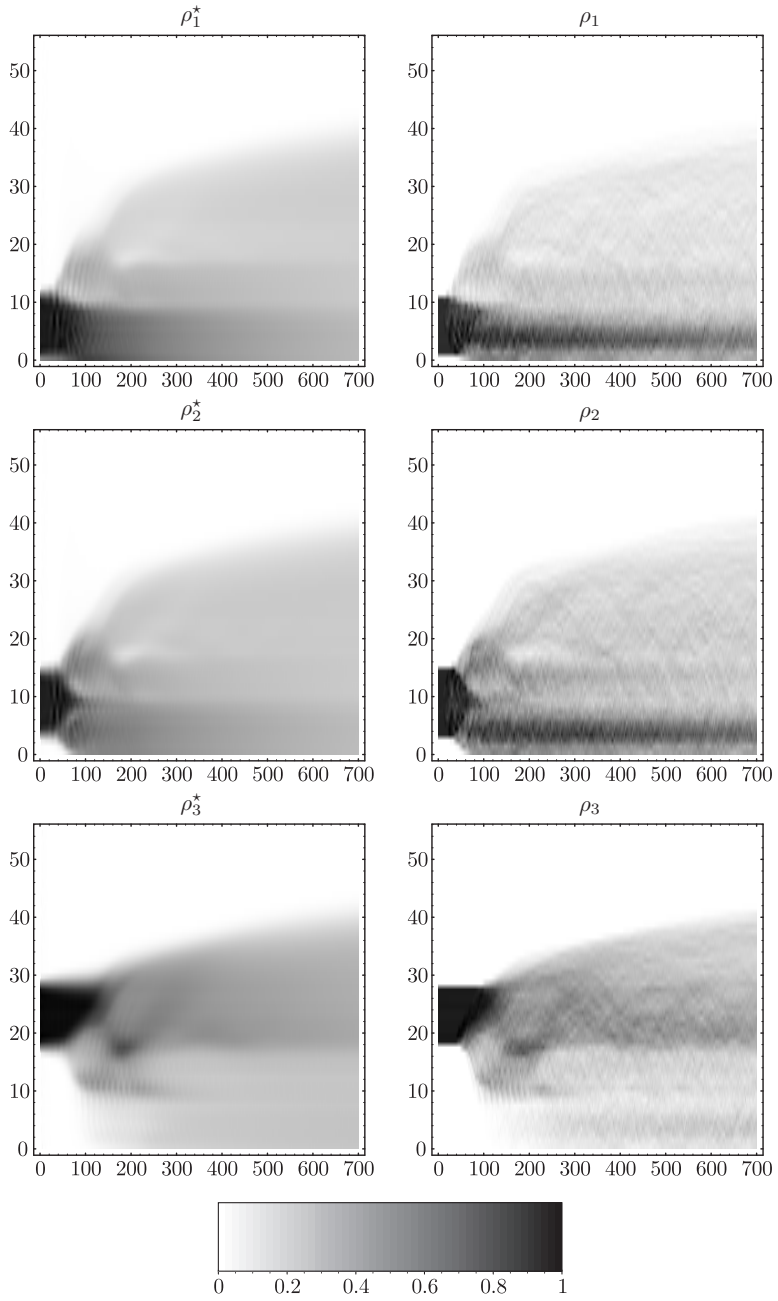

Figure 4. Diffusion indices during the first 7 seconds of the simulation. The horizontal axis represents the time in lattice units (100 = 1second) and the vertical axis represents the layers L_k

where $[b_1,u_1]=[3,12]$, $[b_2,u_2]=[6,15]$, $[b_3,u_3]=[20,29]$. At time $t>0$ we consider a node $\boldsymbol{x}\in T_C$ as a coloured particle when $\delta(\boldsymbol{x},t)>0$. We can thus evaluate the amount of colour in the L_k layer at time t:

$$N_j^\star(t,k)=\sum_{\delta(\boldsymbol{x},t)>0}\delta(\boldsymbol{x},t),\quad k=1,\ldots,54. \tag{30}$$

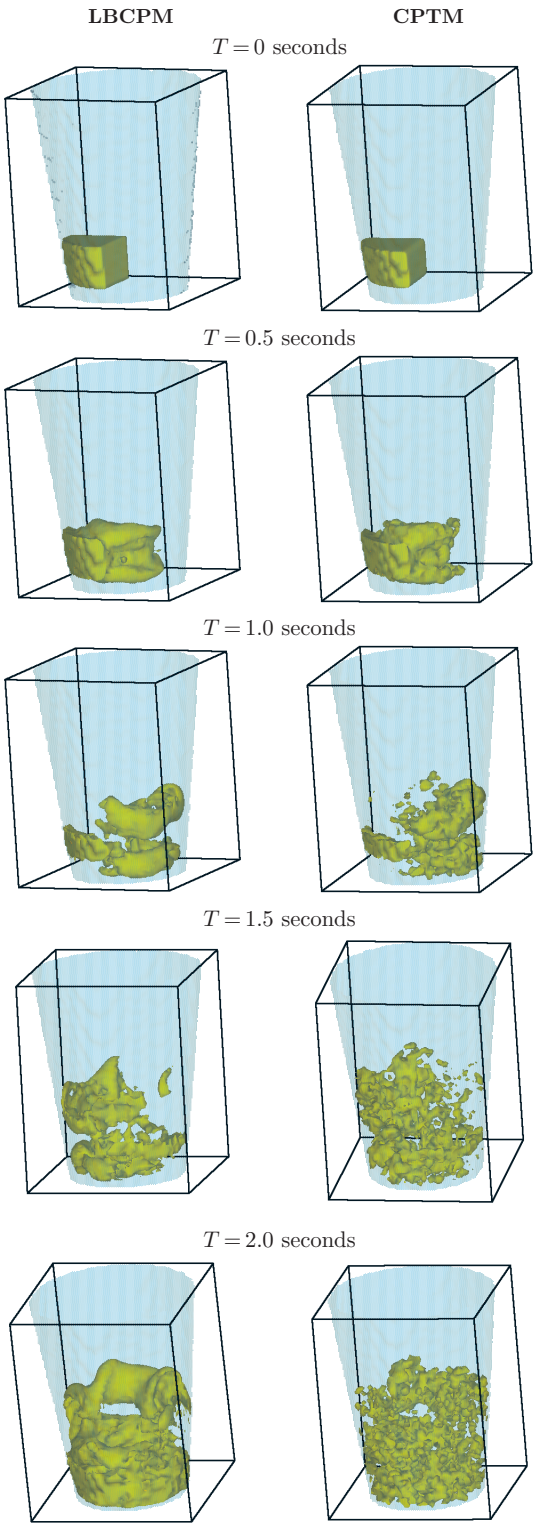

Figure 5. Fluid behaviour in the stirred vessel during the first two seconds of the simulation

Then, we put the diffusion index as:

$$\rho_j^\star(t,k) = \frac{N_j^\star(t,k)}{V_k}, \quad k = 1,\ldots,54, \tag{31}$$

where V_k is the volume of the L_k layer.

In [10] the diffusion index, $\rho_j(t,k)$, is defined as a ratio between $N_j(t,k)$, the number of particles started from the S_j region and arrived in the L_k layer at time t, and V_k:

$$\rho_j(t,k) = \frac{N_j(t,k)}{V_k}, \quad k = 1,\ldots,54. \tag{32}$$

In Figure 4, $\rho_j^\star(t,k)$ and $\rho_j(t,k)$ with $j = 1,2,3$ and $0 \le t \le 7$ seconds are shown. The equality of the $\rho_j^\star(t,k)$ and $\rho_j(t,k)$ indices shows that the diffusive behaviour of the models is very similar.

In Figure 5, we have shown the fluid's qualitative behavior under the action of blades during the first two seconds of the simulations: the results obtained by [10] on the right and the results of the Lattice Boltzmann Coloured Particles Model on the left. As the shapes of the moved fluid and the occupied volume are very similar in both cases, the resemblance of the following images is another proof of the accuracy of the new model.

5. Conclusions

To determine the efficiency of a mixer, one needs to establish means by which the extent of fluid mixing can be gauged both qualitatively and quantitatively. An accurate description of the mixing phenomenon can be achieved by calculating the trajectories of particles in the mixer's flow field from the path equation, $\frac{d\boldsymbol{x}}{dt} = \boldsymbol{u}$. Interpolation of the lattice velocity vectors determines the velocity vector, $\boldsymbol{u}(\boldsymbol{x},t)$, at any point $\boldsymbol{x}$ of the T_C domain. The precision of this model strongly depends on the number of tracked particles, which makes it difficult to parallelize.

To simulate mixing in a stirred vessel, we have developed a new technique, LBCPM, fully based on lattice Boltzmann schemes. We have checked the technique by comparing both the qualitative behaviour and the diffusion indices of the two models. The results show that the two procedures are in good agreement. Furthermore, the run time of LBCPM is comparable to that of the velocity field alone (*cf.* Equations (15), (17) and (22)). The model can be employed efficiently to simulate fluids in a laminar regime only for relatively short time intervals, as problems tend to arise when the simulation time is too long. When the colour function breaks into many components, the colour, due to the intrinsic diffusivity of the model, tend to disappear in the smaller connected components.

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