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

\[ \nabla \cdot \mathbf{u} = 0, \]  
(1)

and by the dimensionless Navier-Stokes equation:

\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla P + \frac{1}{\mathbf{Re}} \nabla^2 \mathbf{u}, \]  
(2)

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

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

\[ \mathbf{Re} = \frac{4l_b^2 \omega_b}{\nu}, \]  
(3)

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

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:

\[ T_C = \left\{ (x_1,x_2,x_3) \in \mathbb{R}^3 : 0 < x_3 < z_s, \ (x_1^2 + x_2^2) < \left( \frac{r_s-r_i}{z_3} \right) x_3 + r_i \right\}, \]  
(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 \( C \):

\[
C = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : z_m \leq x_3 \leq z_M, (x_1^2 + x_2^2) \leq (r_C)^2\},
\]

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 \( 0 < r_C \left(\frac{r_s - r_i}{z_s - z_m} z_m + r_i\right) \).

![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](image)

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 \( \theta_0 \) and \( \theta_2 \) directions produce upward vertical speed while those at \( \theta_1 \) and \( \theta_3 \) produce downward vertical speed (see [14]).

The domain is:

\[
\Omega = T_C \setminus C,
\]

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

\[
\Gamma_0 = \partial T_C, \Gamma_1 = \partial C.
\]

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](image)
We consider the frustum of the right circular cone $T_C$ enclosed in a parallelogram with the following discrete lattice:

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

where $\sigma$ is the minimal distance between two grid points. We set $n_x = 2r_s/\sigma$ and $n_z = zs/\sigma$. Points $x \in T_C$, called active points, define the domain where the simulation takes place, whereas the boundary condition of the vessel is imposed at points $x \in \partial T_C$. 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, $\rho(x,t)$, is represented by the mass distribution functions $F_i$ as follows:

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

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

$$j(x,t) = \sum_{i=0}^{18} F_i(x,t) c_i = \rho u. \quad (10)$$

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

$$\rho(x,0) = \rho_0, \ x \in T_C,$n_x$$

$$j(x,0) = 0, \ x \in T_C. \quad (11)$$

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

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

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

$$\delta(x,0) = \delta_0, \ x \in S,$n_x$$

$$\delta(x,0) = 0, \ x \in T_C \setminus S. \quad (13)$$

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:

$$W_i = \frac{1}{3} \quad i = 0, \quad W_i = \frac{1}{18} \quad i = 1, \ldots, 6,$n_x$$

$$W_i = \frac{1}{36} \quad i = 7, 8, \ldots, 18. \quad (14)$$

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

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

$$F^*_i(x,t+1) = F_i(x,t) + \omega(F^{eq}_i(x,t) - F_i(x,t)), \quad (15)$$

where $F^{eq}_i(x,t)$ is the equilibrium distribution.
and for the colour:

\[ C_i^*(x,t+1) = C_i(x,t) + \lambda_D (C_i^{eq}(x,t) - C_i(x,t)), \]  

(16)

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

\[ F_i^{eq}(x,t) = W_i \rho \left\{ 1 + 3 c_i \cdot u + \frac{9}{2} (c_i \cdot u)^2 - \frac{3}{2} u^2 \right\}, \]  

(17)

\[ C_i^{eq}(x,t) = \frac{\delta(x,t) F_i(x,t)}{\rho(x,t)}. \]  

(18)

The velocity, \( u \), of the fluid is given as follows:

\[ u = \frac{j}{\rho} = \frac{1}{18} \sum_{i=0}^{18} c_i F_i \quad x \in \Omega, \]  

(19)

\[ u = v \quad x \in C, \]

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

\[ \nu = \Delta t c_s^2 \left( \frac{1}{\omega} - \frac{1}{2} \right), \]  

(20)

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

\[ \text{Re} = \frac{4l^2 \omega b}{\nu} = \frac{4l^2 \omega b}{c_s^2 \Delta t \left( \frac{1}{\omega} - \frac{1}{2} \right)} \quad \Rightarrow \quad \omega = \frac{1}{\frac{2}{\nu} + \frac{4l^2 \omega b}{c_s^2 \Delta t \nu}}. \]  

(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:

\[ F_i(x + c_i, t+1) = F_i^*(x, t+1) \quad x \in T_C \cap G_{\sigma}, \]  

\[ C_i(x + c_i, t+1) = C_i^*(x, t+1) \quad x \in T_C \cap G_{\sigma}. \]  

(22)

We apply no-slip conditions on the boundary \( \Gamma_0 \) as in [10].

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

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

(23)

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

\[ P_{ab}(x,t) = \sum_i c_{ia} c_{ib} F_i(x,t) \quad a, b = 1, 2, 3. \]  

(24)

It follows from Equation (23) that, if the value of the relaxation parameter \( \lambda_D \) 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, \( \delta(x,t) \). 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 $x \in G_{\sigma}$ 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 $h = [h_0, \ldots, h_{n-1}]$ such that:

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

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

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

$r_m = r_m(h_i)$ 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 $H_0 = \{x \in G_{\sigma} : 0 \leq x_3 \leq h_0\}$ in the 0 processor, the points of $H_1 = \{x \in G_{\sigma} : h_0 \leq x_3 \leq h_1\}$ 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 $\Omega$ are $r_L = 0.045 \text{ m}$, $r_s = 0.066 \text{ m}$, $z_s = 0.168 \text{ m}$. 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 $\Omega$ domain: its base is $r_s \times r_s$ and its height equals $z_s$. We have considered two discrete grids $G_{\sigma}$ on the parallelepiped. One has a step of $\sigma = 3.0 \cdot 10^{-3} \text{ m}$; 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, $\sigma = 1.5 \cdot 10^{-3} \text{ m}$, 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 $\sigma = 1.5 \cdot 10^{-3} \text{ m}$, the time step is halved.

We consider a fluid with a relatively low Reynolds number: $Re = 250$. The relaxation parameter, $\omega$, is univocally determined by Equation (21). We chose the
Mixing in a Stirred Vessel. A Parallel Implementation...

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):

$$S = \{x \in T_C : z_0 - 0.015 m \leq x_3 \leq z_0 + 0.015 m, 0 \leq x_1, x_2 \leq r_1 \}. \quad (27)$$

Figure 3. Initial position of the coloured particles

The simulations were performed on a cluster made by Xeon at 3.2GHz with Debian as the operating system. They were connected via an Ethernet network at 1Gbit/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 3.2GHz. 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

<table>
<thead>
<tr>
<th></th>
<th>2 processors</th>
<th>4 processors</th>
<th>8 processors</th>
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<tbody>
<tr>
<td>$S_u$</td>
<td></td>
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<tr>
<td>$E_f$</td>
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<tr>
<td>$\sigma = 0.03 m$</td>
<td>1.90</td>
<td>3.22</td>
<td>5.28</td>
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<tr>
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<td>95%</td>
<td>80.5%</td>
<td>66%</td>
</tr>
<tr>
<td>$\sigma = 0.015 m$</td>
<td>1.91</td>
<td>3.44</td>
<td>6.03</td>
</tr>
<tr>
<td></td>
<td>96%</td>
<td>86%</td>
<td>75%</td>
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</table>

4. Results

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

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

where $d_2 = 3.0 \cdot 10^{-3} m$. 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:

$$S_j = \{(x_1, x_2, x_3) \in T_C : b_j \leq x_3 \leq u_j, 0 \leq x_1, x_2 \leq r_1 \}, \quad (29)$$
Figure 4. Diffusion indices during the first 7 seconds of the simulation. The horizontal axis represents the time in lattice units (100 = 1 second) 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 $x \in T_C$ as a coloured particle when $\delta(x, t) > 0$. We can thus evaluate the amount of colour in the $L_k$ layer at time $t$:

$$N^*_j(t, k) = \sum_{\delta(x, t) > 0} \delta(x, t), \quad k = 1, \ldots, 54. \quad (30)$$
Mixing in a Stirred Vessel. A Parallel Implementation...

Figure 5. Fluid behaviour in the stirred vessel during the first two seconds of the simulation
Then, we put the diffusion index as:

$$\rho^j_{\star}(t, k) = \frac{N^j_{\star}(t, k)}{V_k}, \quad k = 1, \ldots, 54,$$

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 $V_k$:

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

(32)

In Figure 4, $\rho^j_{\star}(t, k)$ and $\rho_j(t, k)$ with $j = 1, 2, 3$ and $0 \leq t \leq 7$ 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, $\frac{dx}{dt} = u$. Interpolation of the lattice velocity vectors determines the velocity vector, $u(x, t)$, at any point $x$ 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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Mixing in a Stirred Vessel. A Parallel Implementation...

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