UNIVERSITÉ DE MONTRÉAL

DÉVELOPPEMENT D'UNE MÉTHODE DE BOLTZMANN SUR RÉSEAU POUR LA SIMULATION D'ÉCOULEMENTS VISQUEUX EN CUVES AGITÉES

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Cette thèse intitulée:

DÉVELOPPEMENT D'UNE MÉTHODE DE BOLTZMANN SUR RÉSEAU POUR LA
SIMULATION D'ÉCOULEMENTS VISQUEUX EN CUVES AGITÉES

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CITATION

Tout petit, je voulais être célèbre et je ne faisais rien pour. À l'école, je m'avérais très vite un élève inexistant. Par goût. J'ai toujours été persuadé – je le suis encore – que les diplômes sont faits pour les gens qui n'ont pas de talent. Malheureusement, il ne suffit pas de ne pas avoir de diplômes pour avoir du talent.

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RÉSUMÉ

La caractéristique principale des écoulements visqueux est leur forte résistance à l'écoulement. Comme la prédominance des forces visqueuses empêche la génération de turbulence, la forme de l'écoulement est principalement affectée par la géométrie du problème, la rhéologie du fluide et la présence de plusieurs phases. La simulation de tels écoulements requiert donc l'utilisation d'un outil numérique capable de traiter précisément les géométries, les rhéologies et les interactions entre les phases. Dans la cadre de cette thèse, l'étude des méthodes numériques a pour objectif d'améliorer la simulation des écoulements visqueux en cuves agitées.

La simulation des écoulements dans les mélangeurs permet de compléter les informations obtenues lors des mesures expérimentales. Par exemple, les approches numériques permettent de visualiser facilement les écoulements à l'intérieur du système de mélange, ainsi que de caractériser des grandeurs globales comme le pompage. Pour autant, les résultats ne sont intéressants que si l'on maitrise l'impact des différents paramètres numériques sur la précision. Le cas des mélangeurs industriels spécialisés pour les liquides visqueux concentre un très grand nombre de difficultés. Premièrement, la géométrie du système de mélange est complexe et évolue au cours du temps. En effet, ce type de mélangeur utilise des formes de pales complexes afin de réaliser le mélange. De plus, les pales doivent racler la cuve pour prévenir la stagnation du liquide, ce qui crée des espacements faibles comparativement à la taille du système. Deuxièmement, les propriétés physiques du mélange sont généralement compliquées. La difficulté réside ici dans la modélisation de l'interaction entre les phases ou entre les différents liquides. Dans le cas de l'étude de l'agitation, caractérisée par la simulation d'une seule phase liquide homogène, la difficulté se concentre sur la rhéologie du liquide. Dans le cadre de cette thèse, nous nous limiterons à l'étude de l'agitation.

Malgré ces difficultés, plusieurs travaux de recherche ont été effectués sur la simulation du mélange visqueux dans des cuves agitées utilisées dans l'industrie. Il ressort de ces articles que ce sont principalement les méthodes d'éléments et de volumes finis qui sont utilisées. Malgré des simplifications astucieuses pour faciliter le traitement de la géométrie (tels que les changements de repère ou les conditions aux limites immergées), la simulation des systèmes de mélange entraine un compromis entre la précision des résultats et les temps de calcul. Cette contrainte peut devenir un facteur limitant pour des géométries très complexes et/ou des rhéologies largement

non newtoniennes. Cela s'explique principalement par la taille et la complexité du système d'équations obtenu. Ainsi, dans la littérature, les travaux se situant à l'échelle industrielle se limitent généralement à une seule phase liquide. Certaines simulations polyphasiques sont pourtant réalisées, mais souffrent de temps de calcul très importants et/ou d'approximations affectant globalement la précision. Afin de dépasser ces contraintes, il semble pertinent d'utiliser une méthode efficace pour le calcul parallèle et qui permet de traiter facilement des géométries et des rhéologies complexes. C'est pour cette raison que la méthode de Boltzmann sur réseau est utilisée dans cette thèse.

La méthode de Boltzmann sur réseau « lattice Boltzmann method (LBM) », basée sur la théorie cinétique des gaz, part du principe que la simulation du mouvement de particules de fluide à une échelle physique plus petite (mésoscopique), va permettre d'obtenir le comportement macroscopique du fluide. Ainsi, à partir de l'équation de Boltzmann, la solution des équations de Navier-Stokes peut être obtenue. L'avantage de ce schéma numérique est qu'il est explicite et basé sur des calculs simples et locaux, ce qui lui confère une très bonne efficacité pour le calcul parallèle. À l'inverse, ce changement d'échelle physique comporte aussi des inconvénients, comme la difficulté d'imposer des conditions aux limites macroscopiques. Malgré des approximations sur les phénomènes aux frontières, la LBM a été appliquée avec succès pour la simulation d'écoulements en milieux poreux et de suspensions solide-liquide.

L'objectif principal de cette thèse est de développer une méthode de Boltzmann sur réseau efficace pour la simulation d'écoulements visqueux en cuves agitées. Pour ce faire, il est nécessaire d'étudier l'applicabilité des différentes stratégies pour l'imposition des conditions aux limites et de caractériser la précision de la LBM dans le cas de géométries complexes. Finalement, il est aussi intéressant d'étudier l'applicabilité de la LBM pour des rhéologies complexes.

L'article 1 montre que, dans le cas de géométries courbes (Couette cylindrique et mélangeurs), la précision du schéma LBM est largement affectée par le choix de la stratégie d'imposition de conditions aux limites. Par exemple, dans le cas des mélangeurs raclants, l'approche dite des conditions aux limites immergées « immersed boundary method (IBM) » apparait comme étant moins adaptée. À l'inverse, l'approche la plus simple « modified bounce back-rule (MBB) », basée sur la règle du rebond, et l'approche plus élaborée « extrapolation method (EM) », qui

extrapole les populations en fonction de la distance à l'obstacle, donnent la même précision sur les grandeurs caractéristiques des mélangeurs. Cependant, comme seule la stratégie EM permet d'étudier précisément l'impact d'une petite variation de la géométrie, cette approche est sélectionnée pour la suite des travaux.

L'article 2 montre ensuite que la LBM, couplée avec la méthode d'extrapolation, permet d'obtenir une précision adéquate pour la simulation de la consommation de puissance et de la capacité de pompage du système de mélange Maxblend. Elle permet aussi d'étudier l'impact de paramètres géométriques comme l'espacement entre la pale et le fond de la cuve. De plus, dans le cas d'une géométrie variable dans le temps (configuration avec contre-pales), la précision reste bonne même si les vitesses sont perturbées aux alentours de la pale.

Finalement, l'article 3 montre que, sous certaines limitations sur nombre de Reynolds, la LBM peut être utilisée efficacement pour la simulation d'écoulements fortement non newtoniens. Ainsi, dans le cas du système de mélange Maxblend, un modèle rhéologique de type loi de Carreau-Yasuda avec un indice de puissance de 0.05 a pu être simulé sans affecter largement les temps de calcul.

En conclusion, cette thèse a permis de montrer que la LBM peut être utilisée efficacement pour la simulation des écoulements dans les mélangeurs industriels spécialisés pour les liquides visqueux. Il a même été montré que cette approche pouvait être utilisée pour faire de l'optimisation géométrique des systèmes de mélange. De plus, sous certaines contraintes relatives au régime d'écoulement, il a aussi été montré que la LBM permettait de simuler l'agitation de liquides avec des comportements fortement non newtoniens.

ABSTRACT

The major feature of the viscous flow is its resistance to motion. As the viscous forces are dominant the turbulent phenomena disappear, whereby the shape of the flow is determined by the geometry of the problem, the rheology of the fluid and the presence of several phases. In order to simulate such flows, the selected numerical tool used should be capable of accurately managing the geometry, the rheology and interactions between phases. In the scope of this thesis, numerical methods are assessed in order to improve the simulation of viscous flows in stirred tanks.

In the case of mixing systems, computational fluid dynamics (CFD) is a facilitating tool which may be used to supplement experimental measurements. For instance, numerical simulations allow to readily visualize the flow inside the mixer and determine characteristic mixing numbers, such as the pumping capacity. However, simulation results are useful only if the impact of the numerical parameters on the accuracy is understood. Batch mixers for highly viscous fluids are quite tricky, rendering the simulation process highly challenging. First, the geometry of the mixing system is complex and time dependent. The complex shape of the geometry is though necessary and used to compensate the impossibility of achieving adequate mixing with the turbulence. Given that close clearance impellers are used to prevent the fluid stagnation near the tank, small gaps are found between the tank and impeller. Second, the physical properties of the mixture are also complex. The modelling approach should be able to account for the interaction between the phases (solid, liquid or gas). In the case of blending, only one single liquid phase is considered, thus the difficulty is concentrated on the rheology of the fluid. In this thesis, only blending will be examined.

Notwithstanding such difficulties, the simulation of viscous mixing in stirred tanks has been the subject of many articles. It can be inferred from the literature that the finite element method (FEM) and finite volume method (FVM) have been the most commonly used approaches. Despite the use of ingenious ways to treat the complexity of the geometry (change of reference frame or immersed boundary conditions), the simulation of industrial mixing flows leads to a compromise between accuracy and computation time. This can be explained by the size and complexity of the system of equations to be solved. This limitation can be rather restrictive in the case of particularly complex geometries or highly non-Newtonian behaviors. For instance, most simulations of industrial mixing process consider only one single liquid phase. Conversely, few

multiphase simulations have been applied and suffer from considerable computational cost and/or approximations affecting the accuracy of the simulation. In order to go beyond these limitations, it seems pertinent to use a numerical approach efficient for massive parallel computations. In addition, this method must be able to easily integrate complex geometries and rheology. For the above reasons, the lattice Boltzmann method has been selected in this work.

The lattice Boltzmann method (LBM) is based on the kinetic theory of gas. The idea behind this approach is to obtain the macroscopic dynamics of a fluid from the simulated motion of mesoscopic fluid particles. The solution of the Navier-Stokes equations is then recovered from the Boltzmann equation. As the LBM is explicit and only requires simple and local computations, the resulting scheme is highly efficient for parallel computations. Inversely, the change in physical scale behind the LBM leads to several difficulties, such as the imposition of macroscopic boundary conditions. Despite approximations on the phenomena at the boundaries, the LBM has been successfully applied for the simulation of porous media flows and solid-fluid suspensions.

The main objective of this thesis is to develop an efficient lattice Boltzmann method for the simulation of viscous flows in stirred tanks. To do so, the applicability of the different strategies to impose boundary conditions is first compared. Second, the accuracy of the LBM in the case of complex geometry is characterized. Lastly, the applicability of the LBM for highly non-Newtonian fluid is investigated.

Article 1 illustrates that the accuracy of the scheme is largely affected by the selection of the boundary condition strategy. For instance, in the case of close clearance impellers, the immersed boundary method (IBM) seems to be less accurate. Inversely, the simplest approach, the modified bounce-back rule (MBB), and a more elaborate method, the extrapolation method (EM), which uses the distance from the obstacle to extrapolate missing populations, provide a similar accuracy on characteristic mixing numbers. However, only the EM allows investigating variations of the geometry lower than the lattice spacing. For this reason, this boundary condition strategy is used in the other articles.

Article 2 shows that the LBM accurately predicts the power consumption and pumping capacity of a mixing system. In addition, the impact of geometrical parameters, such as bottom clearance,

can likewise be effectively investigated. Moreover, in the case of time dependent geometries, the LBM conserves an acceptable accuracy even if perturbations appear near the impeller.

Lastly, article 3 demonstrates that, under constraint on the maximum Reynolds number, the LBM can be used to simulate highly non-Newtonian fluid flows. For instance, a Carreau-Yasuda model with a power index of 0.05 was used without largely affecting the computational cost of the simulation.

In conclusion, this thesis has permitted to verify the degree of efficiency and utilization of the LBM for the simulation of viscous flows in stirred tanks. It has also shown that this approach can be used for the optimisation of process geometry. Moreover, under some limitations of the Reynolds number, it can be extended to the blending of highly non-Newtonian fluids.

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Abréviations

BC   Conditions aux limites « *Boundary conditions* »

BGK   Modèle de collision de Bhatnagar, Gross et Krook

CFD   Calcul de la dynamique des fluides « *Computational fluid dynamics* »

DHR   Ruban hélicoïdal double « *Double helical ribbon* »

DNS   Simulation numérique directe « *Direct numerical simulation* »

DPM   Modèle des particules discrètes « *Discrete particle method* »

EM   Méthode d'extrapolation « *Extrapolation method* »

FEM   Méthode des éléments finis « *Finite element method* »

FVM   Méthode des volumes finis « *Finite volume method* »

IB-LBM   Conditions immergées pour la méthode de Boltzmann sur réseau « *Immersed boundary-lattice Boltzmann method* »

IBM   Conditions aux limites immergées « *Immersed boundary method* »

LBGK   Équation de Boltzmann avec le modèle de collision BGK

LBM   Méthode de Boltzmann sur réseau « *Lattice Boltzmann method* »

MBB   Règle du rebond modifiée « *Modified bounce-back* »

MRT   Modèle de collision à plusieurs facteur de relaxation *« Multi Relaxation Time »*

NSERC   *« Natural Sciences and Engineering Research Council of Canada »*

PIV   Vélocimétrie par imagerie de particules « *Particle Image Velocimetry* »

RANS   Équations de Navier-Stokes moyennées « *Reynolds average Navier-Stokes* »

SHI   Sumitomo Heavy Industries

URPEI   Unité de Recherche en Procédés d'Écoulements Industriels

Lettres latines

$\boldsymbol{A}$	Matrice des poids	
a	Paramètre rhéologique de transition du modèle de Carreau-Yasuda	
$\vec{b}$	Vecteur objectif	$m.s^{-1}$
c	Espacement entre la pale et le fond de la cuve	m
c_0	Espacement standard entre la pale et le fond de la cuve	m
c_s	Vitesse du son de lattice	$m.s^{-1}$
D	Diamètre de l'agitateur	m
d	Dimension du problème	
$\vec{e}$	Vecteur vitesse	$m.s^{-1}$
$\vec{e}_k$	Direction ou vecteur vitesse	$m.s^{-1}$
$\vec{e}_i^{(ex)}$	Direction d'extrapolation	$m.s^{-1}$
e	Erreur par rapport à la solution analytique	
F_r	Nombre de Froude	
F_k	Force volumique	$kg.m^{-3}.s^{-1}$
f et f_k	Populations de particules	$kg.m^{-3}$
$f^{(eq)}$ et $f_k^{(eq)}$	Populations d'équilibre	$kg.m^{-3}$
$f_k^{(neq)}$	Population de non équilibre	$kg.m^{-3}$
f_k^{+}	Population de post-collision	$kg.m^{-3}$
G	Fonction d'interpolation	
$\vec{g}$	Force volumique	$N.m^{-3}$
h	Hauteur de liquide	m
$\boldsymbol{I}$	Tenseur identité	

$\vec{J}$	Vecteur de quantité de mouvement	$Kg.m.s^{-1}$
K_n	Nombre de Knudsen	
K_p	Constante de puissance	
K_s	Constante de Meztner-Otto	
k	Numéro de direction,	
k_B	Constante de Boltzmann ($1.381 * 10^{-23}$)	$J.K^{-1}$
L	Dimension caractéristique	m
l	Libre parcours moyen d'une particule	m
M_a	Nombre de Mach	
m	Paramètre rhéologique du modèle de puissance	$Pa.s^{2-n}$
N	Vitesse de rotation de l'agitateur	RPS
N_p	Nombre de puissance	
N_q	Nombre de pompage	
n	Indice de puissance des modèles rhéologiques	
P	Puissance consommée	W
p	Pression	Pa
Q_z^+	Débit caractéristique	$m^3.s^{-1}$
q	Nombre de directions par lattice	
R	Constante des gaz parfaits	$J.mol^{-1}.K^{-1}$
Re	Nombre de Reynolds	
Re_g	Nombre de Reynolds généralisé	
r	Rayon	m
r_{in}, r_{out}	Rayons de cylindre	m
$\boldsymbol{S}$	Tenseur du taux de déformation	s^{-1}

$\vec{s}$	Coordonnées paramétriques	m
T	Température	K
t	Coordonnée temporelle	s
t_+	Temps post-collision	s
t_m	Temps de mélange	
$\vec{u}$	Vecteur vitesse	$m.s^{-1}$
$\vec{u}_b$	Vitesse de l'obstacle	$m.s^{-1}$
$\vec{u}_c$	Vitesse des points de contrôle	$m.s^{-1}$
$\vec{u}_f$	Vitesse d'une lattice fluide	$m.s^{-1}$
$\vec{u}_{ff}$	Vitesse d'une lattice voisine fluide	$m.s^{-1}$
$\vec{u}_w$	Vitesse extrapolée à une lattice solide	$m.s^{-1}$
V	Capacité de la cuve	L
$\vec{X}_c$	Coordonnées des points de contrôle	m
$\vec{x}$	Coordonnées spatiales	m
$\vec{x}_b$	Coordonnées d'un point de la frontière	m
$\vec{x}_c$	Coordonnées du centre de gravité	m
$\vec{x}_f$	Coordonnées d'une lattice fluide	m
$\vec{x}_{ff}$	Coordonnées d'une lattice voisine fluide	m
$\vec{x}_w$	Coordonnées d'une lattice solide	m

Lettres grecs

Γ	Frontière du domaine	
Δ	Distance à l'obstacle	
ΔS_i	Unité de surface	m^2

Ω	Opérateur de collision	
β	Paramètre d'extrapolation	
$\dot{\gamma}$	Taux de cisaillement	s^{-1}
$\dot{\gamma}_c$	Taux de cisaillement caractéristique	s^{-1}
γ_i	Paramètre d'extrapolation	
δ_{ij}	Fonction de Kronecker	
δt	Pas de temps	s
δx	Pas d'espace ou taille de lattice	m
ε	Énergie interne	J
ϵ	Paramètre de la décomposition de Chapman-Enskog	
η ou μ	Viscosité dynamique du fluide	$Pa.s$
η_0	Viscosité à cisaillement nul	$Pa.s$
η_∞	Viscosité à cisaillement infini	$Pa.s$
λ	Temps caractéristique pour le modèle de Carreau-Yasuda	s
ρ	Masse volumique du fluide	$kg.m^{-3}$
ρ_0	Masse volumique moyenne du fluide	$kg.m^{-3}$
$\boldsymbol{\sigma}$	Tenseur des contraintes	Pa
τ	Facteur de relaxation	
τ_0	Facteur de relaxation de référence à taux de cisaillement nul	
$\vec{\varphi}$	Vecteur de corrections des vitesses	$m.s^{-1}$
ω	Poids des polynômes Hermitiens	
ω_k	Poids des populations	

Symboles

∇	Gradient	
∂_t	Dérivée temporelle	

Exceptions relatives aux articles

Article 1 :

D	Diamètre de la cuve	m
d	Diamètre de l'agitateur	m
Ω	Domaine de simulation	
$\dot{\boldsymbol{\gamma}}$	Tenseur du taux de déformation	s^{-1}
ε	Tolérance	
$\boldsymbol{\tau}$	Tenseur des contraintes	Pa
ω	Vitesse de rotation	s^{-1}

Article 2 :

$\vec{F}, \vec{F}_k$	Force	N
G_k	Force volumique	$kg.m^{-3}.s^{-1}$
H	Hauteur de liquide	m
n	Nombre total de lattices fluides	
T	Diamètre de la cuve	m
W	Largeur des contre-pales	m
Ω	Domaine de simulation	
$\dot{\boldsymbol{\gamma}}$	Tenseur du taux de déformation	s^{-1}
ω	Vitesse de rotation	s^{-1}

Article 3 :

F	Hauteur de pale	m
H	Hauteur de liquide	m
T	Diamètre de la cuve	m
W	Largeur des contre-pales	m
ω	Vitesse de rotation	s^{-1}

LISTE DES ANNEXES

CHAPITRE 1   INTRODUCTION

1.1   Contexte

Ce travail au sein du laboratoire de l'Unité de Recherche en Procédés d'Écoulements Industriels (URPEI) s'inscrit dans la problématique associée à l'étude des écoulements complexes dans les cuves agitées. Dans ce laboratoire, les méthodes expérimentales et numériques sont utilisées pour améliorer la compréhension des phénomènes associés aux écoulements polyphasiques et aux rhéologies complexes survenant dans les géométries possédant des parties mobiles ou des formes complexes.

La méthode numérique la plus couramment utilisée à l'URPEI pour la simulation d'écoulements visqueux est la méthode des éléments finis (FEM). Grâce à cette approche, la caractérisation des écoulements de nombreux mélangeurs a été réalisée dans les régimes laminaires et transitoires. Ces résultats ont été obtenus grâce à plusieurs travaux de recherche traitant de la modélisation de la complexité de la géométrie. Dans la majorité des cas, les simulations se limitent à l'agitation d'un liquide unique dont les propriétés rhéologiques restent relativement simples.

Cette thèse s'inscrit donc dans l'objectif à long terme de simuler des écoulements polyphasiques et à rhéologies complexes dans des cuves agitées. L'idée principale est de tirer profit des particularités de la méthode de Boltzmann sur réseau (LBM) pour faciliter la modélisation de la complexité de la géométrie et des écoulements. L'utilisation de cette méthode est motivée par les résultats obtenus par un code LBM, développé à l'URPEI, pour la simulation numérique directe d'écoulements dans des milieux poreux [1-3]. Ces travaux de recherche ont montré les grandes capacités de la LBM pour le calcul en parallèle et la facilité à traiter des géométries complexes.

Finalement, il est important de souligner que les conclusions de cette thèse ne se limitent pas à la simulation des écoulements en cuves agitées, mais sont applicables à tous problèmes comprenant des écoulements visqueux dans des géométries complexes avec des parties mobiles.

1.2 Les écoulements visqueux complexes

Les écoulements visqueux complexes font référence à des écoulements caractérisés par une prédominance des termes visqueux sur l'inertie, empêchant ainsi la création de turbulence. Les différentes sources de complexité peuvent se trouver dans la géométrie, la rhéologie du fluide ou la présence de plusieurs phases. Dans le cadre de cette thèse, dont l'application concerne les écoulements visqueux en cuves agitées, nous étudierons principalement la problématique du traitement de la complexité de la géométrie. Dans la dernière partie, l'impact de la rhéologie sera aussi étudié.

1.2.1 Les écoulements dans des géométries complexes

L'écoulement dans un milieu poreux est un exemple très connu d'écoulement visqueux complexe. Comme illustré dans la Figure 1.1, la surface de contact entre le fluide et le solide est très grande et de forme complexe.
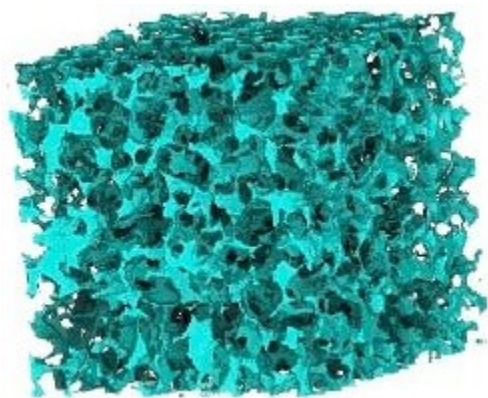
Figure 1.1: Espace poreux d'un morceau de grès [4].

Avec les méthodes standards de CFD, la discrétisation de la partie fluide est très difficile à réaliser et génère un très grand nombre d'éléments (ou de cellules), ce qui complique le calcul de la solution. Afin de contourner cette difficulté, il est possible de modéliser l'action du milieu poreux sur le fluide par un modèle de Darcy [5]. L'introduction d'un modèle supplémentaire entraine une réduction de la précision des simulations, mais permet d'obtenir un résultat dans un temps de calcul raisonnable (voir un exemple d'applications dans [6]). À l'inverse, l'utilisation de la LBM facilite grandement la simulation numérique directe de l'écoulement dans un milieu poreux. En effet, à l'aide d'un maillage structuré cubique et d'une approximation des frontières

par faces, l'étape de discrétisation devient possible [1]. Comme la méthode est explicite et très efficace pour le calcul parallèle, elle permet d'utiliser un très grand nombre d'éléments (lattices) [3]. Par exemple, l'utilisation de la LBM a permis la simulation numérique directe de l'écoulement dans un pot catalytique à l'aide de 3.6×10^9 lattices fluides [7], comme illustré dans la Figure 1.2.
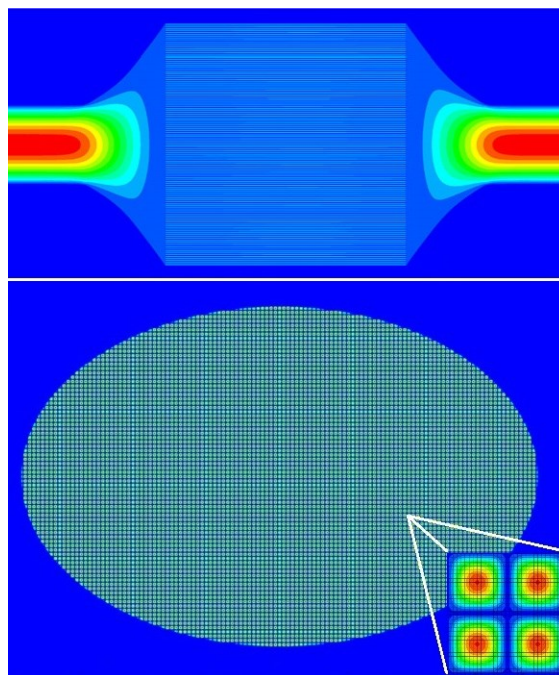
Figure 1.2: Simulation LBM dans un pot catalytique (tirée de [7])

Les géométries avec parties mobiles ajoutent une degré supplémentaire de difficulté puisqu'il est nécessaire d'adapter la discrétisation en fonction du mouvement des objets. Comme la reconstruction du maillage dans le temps est une tâche très difficile et très longue, ce sont les méthodes de maillages glissants [8] ou de conditions aux limites immergées [9, 10] qui sont préférées. Ce point sera traité plus en détail dans la section 1.3.3 pour le cas des cuves agitées.

1.2.2 Les modèles rhéologiques

L'écoulement d'un fluide dans une géométrie donnée est très largement affecté par sa rhéologie, il est donc important de modéliser précisément ses effets. Comme dans le cas général la valeur de la viscosité d'un fluide dépend d'un très grand nombre de paramètres, le but de la rhéologie est de caractériser les dépendances les plus significatives afin de modéliser le comportement des

fluides. Dans le cadre de cette thèse, l'utilisation des modèles sera restreinte aux comportements newtoniens et pseudo-plastiques.

Dans le cas des fluides newtoniens et non newtoniens sans effet d'élasticité, la relation entre le tenseur des contraintes $\boldsymbol{\sigma}$ et le tenseur du taux de déformation $\boldsymbol{S}$ est définie comme :

$$\boldsymbol{\sigma} = p\boldsymbol{I} - 2\eta\boldsymbol{S} \tag{1.1}$$

avec p la pression, η la viscosité dynamique, $\boldsymbol{I}$ le tenseur identité et $\boldsymbol{S} = (\nabla\vec{u} + \nabla^T\vec{u})/2$.

Dans le cas newtonien, la viscosité est constante ($\eta = \mu$). Dans le cas non newtonien, elle est fonction du taux de cisaillement $\dot{\gamma} = \sqrt{2\boldsymbol{S}:\boldsymbol{S}}$. Les comportements les plus courants sont représentés dans la Figure 1.3(a). Afin de décrire un comportement pseudo-plastique (ou rhéofluidifiant), le modèle le plus simple est la loi de puissance [11] :

$$\eta = m\dot{\gamma}^{n-1} \tag{1.2}$$

où les paramètres m et n sont déterminés empiriquement.

Afin de corriger le modèle aux valeurs limites du taux de cisaillement ($\lim_{|\dot{\gamma}|\to 0}\eta = \infty$ et $\lim_{|\dot{\gamma}|\to\infty}\eta = 0$), il est possible d'utiliser le modèle de Carreau-Yasuda [11] :

$$\frac{\eta - \eta_\infty}{\eta_0 - \eta_\infty} = [1 + (\lambda\dot{\gamma})^a]^{\frac{n-1}{a}} \tag{1.3}$$

avec η_0 et η_∞ les viscosités à taux de cisaillement nul et infini, λ le temps caractéristique et a un paramètre qui décrit la transition entre le comportement newtonien et la loi de puissance. Ce modèle permet d'inclure deux plateaux newtoniens aux valeurs limites du taux de cisaillement, comme illustré dans la Figure 1.3(b).

Dans le cas général, l'intégration d'un modèle rhéologique dans les équations de Navier-Stokes rend leur résolution plus difficile [12]. Par exemple, il a été montré que lors de l'utilisation d'un modèle de loi de puissance, il est très difficile de simuler un liquide avec un indice de puissance $n < 0.3$ [13]. Dans le cas de la LBM, l'intégration d'un modèle rhéologique sans effet d'élasticité peut se faire d'une manière naturelle qui ne perturbe pas les propriétés du schéma

[14]. Par exemple, on notera des simulations réalisées avec des modèles de loi de puissance [15, 16] et de Carreau-Yasuda [17, 18]. Ce point sera traité plus en détail dans la section 2.5.
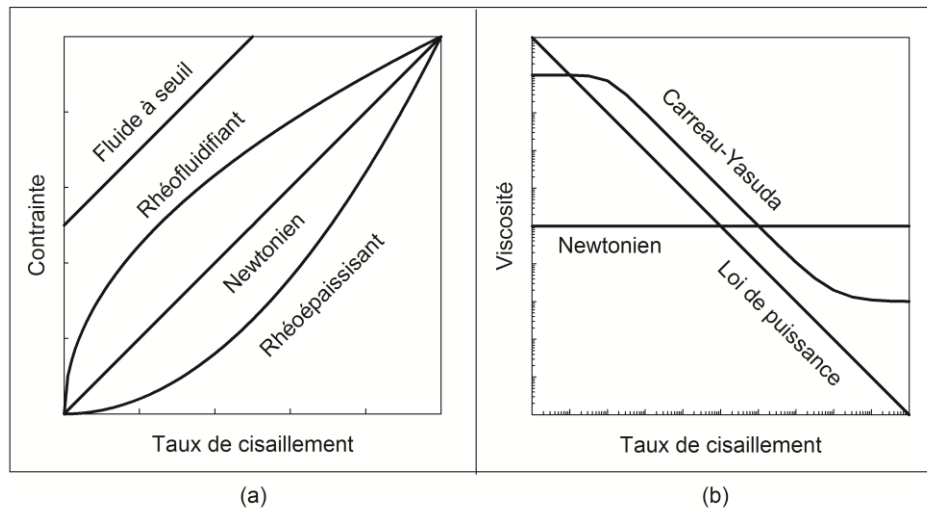
Figure 1.3: Illustrations des comportements rhéologiques

1.2.3 Les écoulements polyphasiques

Dans le cadre de cette thèse, les écoulements polyphasiques ne seront pas étudiés. Cependant, il est intéressant d'aborder cette problématique puisqu'elle s'inscrit dans la continuité de ce travail.

Afin de réaliser la simulation directe d'un écoulement polyphasique, les problématiques soulevées précédemment reviennent. En effet, pour décrire adéquatement l'interaction entre les phases, il est nécessaire de discrétiser précisément la frontière qui les sépare, comme illustré dans la Figure 1.4 dans le cas d'une suspension. De la même façon, la rhéologie des fluides en présence va affecter largement l'écoulement global.
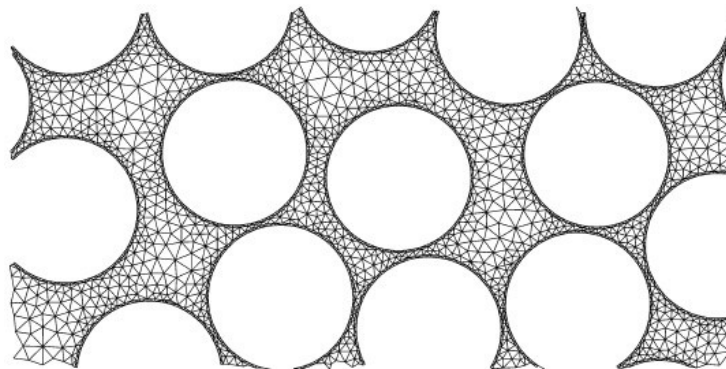
Figure 1.4: Discrétisation d'une suspension (simulation 2D) [19]

Comme il n'est généralement pas réalisable d'effectuer une simulation numérique directe (DNS) d'un écoulement polyphasique à l'échelle industrielle, il est nécessaire de modéliser certains phénomènes physiques au sein de l'écoulement. Le choix de la méthode et des modèles utilisés est un compromis entre la taille de la discrétisation et l'échelle physique étudiée. Le lecteur intéressé pourra se référer à [20] pour un exemple de stratégie multi-échelle appliquée à la simulation de lits fluidisés gaz-liquide. En fonction de l'échelle physique désirée, il est possible d'utiliser des méthodes continues monophasiques (ou 1-fluide) [21, 22], dont les propriétés du fluide modèle doivent caractériser l'écoulement polyphasique au complet, ou des méthodes continues avec 2 fluides [23-25] qui permettent de modéliser l'écoulement polyphasique comme l'enchevêtrement de deux fluides. Il est à noter que l'augmentation des capacités de calcul a permis l'application de stratégies de simulation à l'échelle intermédiaire, comme celle des particules discrètes (DPM) [26-28] dans le cas des suspensions. Avec cette approche, il y a un couplage entre les particules et le liquide, c'est-à-dire que le liquide agit sur les particules et que celles-ci agissent aussi sur le liquide. Les trajectoires des particules sont déterminées grâce à la seconde loi de Newton (approche Lagrangienne) et les collisions sont modélisées (voir [29, 30] pour un modèle de type ressort-amortisseur). Contrairement à la DNS, la phase liquide est continue dans tout le domaine (pas de frontière avec les particules), ce qui permet de réduire le nombre d'éléments utilisés et donc les temps de calcul.

1.3   Le mélange visqueux en cuves agitées

Les mélangeurs sont couramment utilisés dans l'industrie dans le but de disperser une substance, de mélanger plusieurs phases ou de conserver l'homogénéité d'une mixture. Les mélangeurs industriels présentent une large variété de formes et de fonctionnements afin de s'adapter à toutes les situations. Que les systèmes de mélange soient dynamiques ou statiques, qu'ils utilisent des pales raclantes ou des hélices, ils profitent de l'écoulement en leur sein pour réaliser ou conserver le mélange de produits.

D'une manière générale, la façon la plus rapide et la plus simple de mélanger est d'utiliser la turbulence. En effet, grâce à l'action des tourbillons présents aux différentes échelles, l'enchevêtrement des différents produits est rapidement réalisé. À l'inverse, dans le cas des liquides visqueux, la turbulence ne peut être utilisée car elle entrainerait une consommation d'énergie trop élevée. Le mélange visqueux est expliqué plus en détails dans la section suivante.

1.3.1 Les géométries des mélangeurs

Les mélangeurs spécialisés pour les liquides visqueux compensent l'impossibilité d'utiliser la turbulence par des géométries complexes. Par exemple, la Figure 1.5 présente 3 types de mélangeurs : un mélangeur statique, un mélangeur planétaire et un mélangeur raclant.
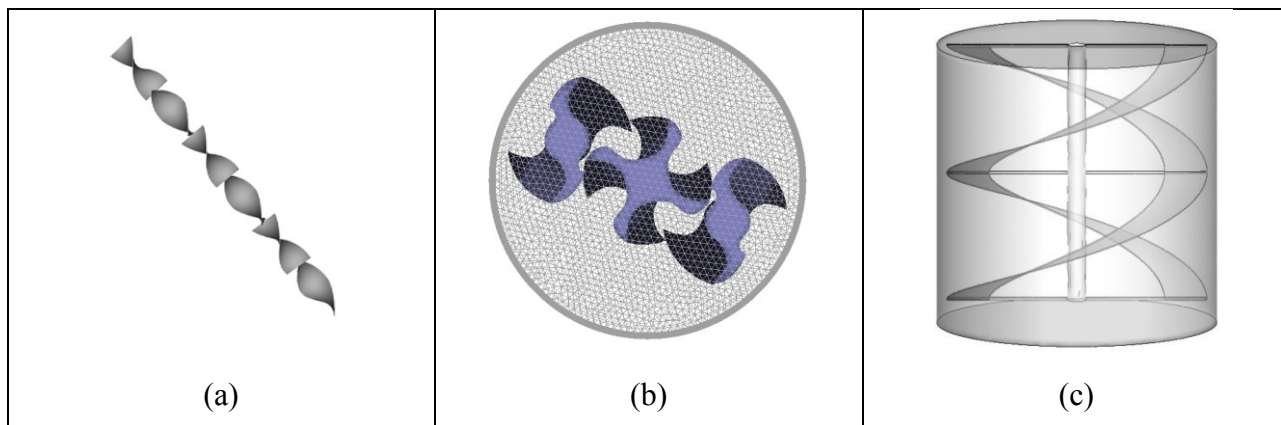
Figure 1.5 : Exemples de mélangeurs spécialisés pour les liquides visqueux : (a) mélangeur statique Kenics, (b) mélangeur planétaire tripale et (c) double ruban hélicoïdal.

Dans ces trois exemples, la géométrie des obstacles ou des parties mobiles a pour but de plier et d'étirer les lignes de courant afin de générer le mélange. Autrement dit, l'efficacité d'un mélangeur spécialisé pour les liquides visqueux se caractérise par sa capacité à créer du cisaillement (ou de l'élongation). D'un point de vue industriel, il est important que ce cisaillement soit réalisé à moindre coût. La notion du coût de mélange est généralement abordée à partir de la consommation de puissance du système de mélange.

Dans cette thèse, ce sont les mélangeurs discontinus « batch mixer » spécialisés pour les liquides visqueux qui sont étudiés. Ils sont caractérisés par la présence d'une cuve et d'au moins un agitateur, comme présenté dans la Figure 1.6, et sont très largement utilisés pour les procédés de fabrication qui nécessitent plusieurs phases. Pouvant être associés à un système de contrôle de la température, ils permettent aussi bien de contrôler l'homogénéité d'une mixture durant toute la durée du procédé que de disperser un additif. Ces systèmes doivent être capables de prévenir toutes stagnations du produit ou toutes créations de zones mortes. Pour ce faire, les pales doivent racler le bord et le fond de la cuve et être capables de générer une circulation axiale. Ultimement, un système de mélange spécialisé pour les fluides visqueux doit être capable de générer un fort

cisaillement (mélange dispersif) et une circulation axiale dans tout le volume de la cuve (mélange distributif).

Figure 1.6: Mélangeur Maxblend (SHI, 2008)

L'efficacité du mélange est aussi largement affectée par les propriétés physiques de la mixture. Par exemple, un système très efficace pour des liquides newtoniens peut voir ses performances diminuer largement pour des rhéologies complexes. D'une manière générale, le choix d'un système de mélange est basé sur la situation la plus problématique, c'est-à-dire la phase du procédé où la viscosité est la plus élevée ou lorsque que la rhéologie est la plus complexe.

1.3.2 Les grandeurs caractéristiques des mélangeurs

Afin de comparer les systèmes de mélange entre eux, trois critères peuvent être utilisés : le temps de mélange, la consommation de puissance et le pompage. L'utilisation de ces grandeurs reste limitée car elles dépendent du régime de l'écoulement, de la rhéologie et des paramètres géométriques.

Dans le cas d'un système de mélange avec une seule pale, le nombre de Reynolds est défini comme :

$$Re = \frac{\rho N D^2}{\mu} \tag{1.4}$$

avec ρ la masse volumique du fluide, N la vitesse de rotation et D le diamètre de l'agitateur.

Cette définition peut être généralisée aux cas non newtoniens. Dans le cas d'un liquide pseudo-plastique, le concept de Metzner et Otto [31] propose de définir la viscosité caractéristique à l'aide du taux de cisaillement $\dot{\gamma}_c = K_s N$, K_s étant une constante qui dépend seulement de la géométrie du système. Le nombre de Reynolds généralisé est donc :

$$Re_g = \frac{\rho N D^2}{\eta(K_s N)} \qquad (1.5)$$

Le temps de mélange est une notion prépondérante pour la comparaison des mélangeurs car il permet de caractériser le temps nécessaire pour obtenir l'homogénéité du mélange. Cette grandeur peut être mesurée expérimentalement grâce à des méthodes de décoloration [32, 33]. Le principe est basé sur l'injection d'un réactif qui modifie les propriétés visuelles du mélange. Ainsi, pour chaque nombre de Reynolds étudié, le temps de mélange t_m est atteint quand le réactif a agi sur le volume complet du fluide. De cette manière, il est possible de construire des courbes Nt_m versus Re afin de comparer les systèmes de mélange. Par exemple, la Figure 1.7 montre que les rubans hélicoïdaux présentent un temps de mélange faible pour des régimes très laminaires ($Re < 10$), à l'inverse ce sont les turbines qui sont les plus performantes à hauts nombres de Reynolds.
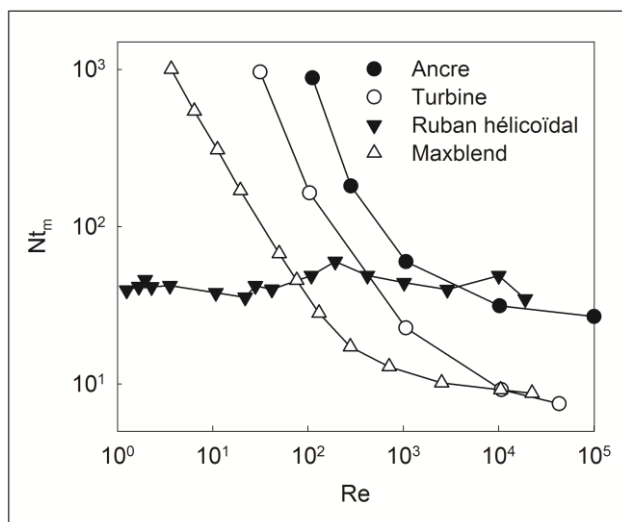
Figure 1.7: Courbes de temps de mélange pour différents systèmes d'agitation (données provenant de Yamato et al., 1998 [34])

Le coût du mélange est généralement caractérisé à travers la consommation de puissance P du système d'agitation. Pour ce faire, le nombre adimensionnel de puissance N_p est défini comme :

$$N_p = \frac{P}{\rho N^3 D^5} \tag{1.6}$$

Ce nombre est constant dans le régime turbulent, comme illustré dans la Figure 1.8 dans le cas du mélangeur Maxblend. À l'inverse, en régime laminaire, c'est la constante adimensionnelle de puissance $K_p = N_p.Re$ qui est constante. On remarque que grâce au concept de concept de Metzner et Otto introduit à la page précédente, il est possible de superposer les courbes de puissance newtonienne et non newtonienne.
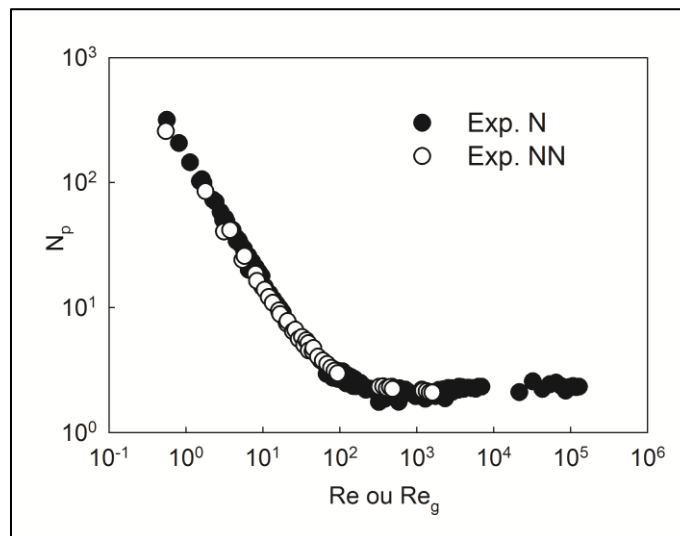
Figure 1.8: Courbes de puissance pour le mélangeur Maxblend (données provenant de Guntzburger et al., 2012 [35]).

La création d'une circulation axiale dans le système de mélange est cruciale pour l'homogénéité de la mixture. Afin de mesurer la capacité de pompage, le nombre de pompage N_q est défini comme :

$$N_q = \frac{Q_z^+}{ND^3} \tag{1.7}$$

La valeur du débit caractéristique Q_z^+ est généralement approximée par l'intégration du champ de vitesse passant au travers d'un groupe de plans [13, 36]. La répartition et la forme de ces plans dépendent de la géométrie du système de mélange.

Les valeurs des grandeurs caractéristiques associées au temps de mélange et au pompage peuvent varier avec la rhéologie et donc caractériser un gain ou une perte de performance du système de mélange. Afin d'obtenir les valeurs de t_m, N_p et N_q, il est possible d'utiliser les approches expérimentales et numériques. Chacune possédant des avantages et des inconvénients, il est intéressant d'utiliser les deux approches conjointement afin de maximiser l'information sur un système de mélange.

1.3.3 La simulation du mélange visqueux

L'utilisation des méthodes numériques permet de compléter les informations obtenues grâce aux approches expérimentales. Par exemple, elles permettent facilement de visualiser des écoulements tridimensionnels globaux ou, à l'inverse, d'obtenir des informations locales sans modifier l'écoulement en lui-même. Pour autant, les méthodes numériques possèdent aussi leurs propres limites. Dans le cas du mélange visqueux, les difficultés apparaissent dans le traitement de la géométrie, de la rhéologie et des écoulements polyphasiques.

Dans le cas des mélangeurs discontinus, l'écoulement est généré par le mouvement des pales. Il est donc primordial que la méthode numérique utilisée soit capable de modéliser précisément l'impact de la pale sur le liquide environnent. Cette tâche est non triviale car la géométrie de la pale est complexe et sa position varie dans le temps. Aussi, il n'est pas réalisable de remailler la zone liquide à chaque itération car cela entrainerait des temps de calcul trop importants. Afin de contourner cette difficulté, plusieurs solutions sont disponibles dans la littérature. Premièrement, lorsque que la forme de la géométrie n'évolue pas dans le temps, il est possible d'appliquer un changement de repère, comme présenté dans la Figure 1.9(a). Ainsi, à l'aide d'un repère Lagrangien associé à la pale [37], il est possible de résoudre les équations de Navier-Stokes sur un maillage fixe. Il suffit simplement de corriger les équations en incluant les forces de Coriolis et centrifuge. Malheureusement, cette approche est très limitative car elle ne permet que la simulation d'une pale centrée dans une cuve sans contre-pale. Afin de dépasser cette limitation, il est possible de décomposer le volume en deux parties cylindriques coaxiales (voir Figure 1.9(b)). La première partie, associée au repère naturel, comprend la cuve et les contre-pales. La deuxième

partie, associée à un repère Lagrangien, n'inclut que la pale. De cette manière, il est possible de résoudre les équations de Navier-Stokes dans deux géométries fixes, la difficulté résidant ici dans la définition de la communication entre les zones. Avec à la méthode dite des repères multiples « mutiple reference frame » (voir Brucato et al. [38] pour un exemple d'application), il est possible d'obtenir une approximation stationnaire de l'écoulement. Pour pouvoir obtenir l'évolution de l'écoulement dans le temps, il faut utiliser la méthode du maillage tournant « sliding mesh » [8], qui permet de prendre en compte la rotation de la pale. Cependant, comme il est difficile de gérer les communications entre les deux zones, la précision peut être dégradée [39]. Ces techniques sont difficilement applicables aux agitateurs raclants car elles nécessitent un écart important entre la pale et la cuve. De plus, le mouvement de la pale est limité à une rotation autour de son axe. Afin de dépasser ces limitations, il est possible d'utiliser une méthode de type conditions aux limites immergées « immersed boundary method (IBM) » [9, 10, 40]. Le principe est de considérer un domaine entièrement fluide à l'intérieur duquel, à différents points de contrôle, la vitesse du fluide est contrainte. Ainsi, comme présenté dans Figure 1.9(c), à l'aide d'un groupe de points décrivant la surface de la pale, le fluide environnant est contraint à suivre le mouvement de l'agitateur. Dans ce cas, le traitement de la variation de la géométrie se limite à la simple modification des coordonnées des points de contrôle. Cette méthode est plus générique mais la précision du champ de vitesse autour des points de contrôle n'est pas toujours maitrisée.
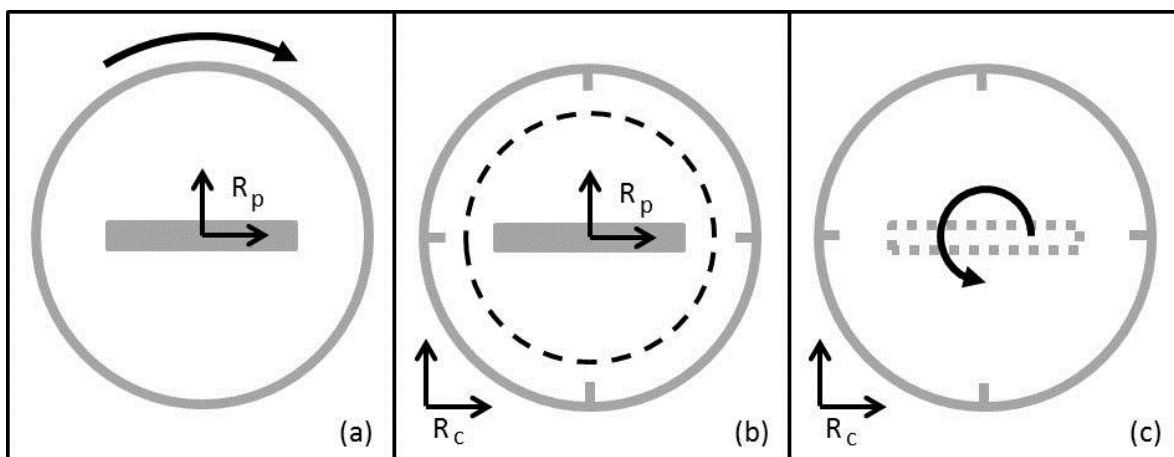
Figure 1.9: Illustrations des différentes approches de gestion de la géométrie. (a) changement de repère, (b) utilisation de deux repères et (c) conditions aux limites immergées. R_c et R_p réfèrent aux repères fixes par rapport à la cuve et à la pale, respectivement.

Grâce à ces différentes approches, des nombreux systèmes de mélanges ont été étudiés. Il ressort de la littérature que c'est principalement la méthode des éléments finis « finite element method (FEM) » qui est utilisée, le plus généralement pour des régimes laminaire et transitoire. Ainsi, grâce à l'utilisation d'un repère Lagrangien, les hydrodynamiques d'un mélangeur Paravisc® [41], d'un malaxeur à pâte [42], de rubans hélicoïdaux (DHR) [12, 37, 43] et d'un mélangeur Maxblend® [13, 36, 43, 44] ont été étudiées avec succès. Pour des géométries plus complexes, les méthodes de type conditions aux limites immergées ont permis de simuler les écoulements dans des mélangeurs planétaires [44, 45] et dans un mélangeur Maxblend avec contre-pales [13, 36, 44]. On notera aussi le couplage d'une méthode de conditions aux limites immergées avec un maillage glissant pour simuler l'hydrodynamique du Superblend® [46], constitué d'un Maxblend et d'un DHR. Pour ce qui est de la rhéologie, la FEM a permis de simuler des comportements pseudo-plastiques avec des modèles de type loi de puissance [13, 41] et Carreau-Yasuda [42], l'indice de puissance le plus petit étant $n = 0.3$. On notera aussi l'utilisation d'un modèle simplifié de comportement viscoélastique [12] et d'un fluide à seuil de type Bingham [47].

Pour la méthode des volumes finis « finite volume method (FVM) », son utilisation dans le cadre du mélange est généralement couplée à la méthode de maillage glissant et se situe dans le régime turbulent. En effet, la plupart des articles sont basés sur l'utilisation du logiciel Fluent®, lequel dispose d'une méthode de type maillage glissant. Ce sont généralement des turbines Rushton qui ont été étudiées [48-51] dans le cas de régimes d'écoulements turbulents (donc faiblement visqueux). Dans le cas d'écoulements à nombres de Reynolds plus faibles, on notera l'étude d'un mélangeur coaxial constitué d'une ancre et d'une turbine [52].

À partir de ces travaux, il apparait que la simulation de l'hydrodynamique au sein des mélangeurs industriels pour liquides visqueux est principalement faite à l'aide de la méthode des éléments finis. Les simulations sont généralement monophasiques (agitation d'un liquide) et se limitent à des rhéologies simples ($n > 0.3$). Ces restrictions s'expliquent par le très grand nombre d'éléments (et donc d'équations) nécessaires pour décrire la complexité de la géométrie. À cela s'ajoute l'intégration de la rhéologie qui, à cause de la non linéarité inhérente à ces modèles, entraine une dégradation des propriétés du système d'équations à résoudre. Ces difficultés mènent généralement à un compromis entre précision et temps de calcul, limitant alors la simulation de problèmes plus complexes, comme le mélange de mixtures polyphasiques ou à

rhéologies complexes. Afin de contourner ces difficultés, il est pertinent de tester de nouvelles approches numériques.

Comme la méthode de Boltzmann sur réseau « lattice Boltzmann method (LBM) » est très efficace en parallèle [2], qu'elle permet de traiter des géométries complexes [3, 53] et d'intégrer facilement des modèles rhéologiques [16, 27, 54], nous proposons de l'utiliser dans le cas des écoulements visqueux en cuves agitées.

1.4 Objectif principal de la thèse

Au regard des difficultés mentionnées précédemment pour la simulation du mélange visqueux, il est maintenant possible de formuler l'objectif principal de cette thèse :

Développer une méthode de Boltzmann sur réseau efficace pour la simulation d'écoulements visqueux en cuves agitées.

L'hypothèse associée à cet objectif est que l'utilisation de la LBM va permettre d'accroitre les possibilités de simulations au travers de la prise en compte efficace de la géométrie et de la rhéologie.

CHAPITRE 2   REVUE DE LITTÉRATURE : MÉTHODE DE BOLTZMANN SUR RÉSEAU

Dans ce chapitre, les aspects fondamentaux de la méthode de Boltzmann sur réseau sont brièvement introduits afin de faire ressortir les notions importantes pour la simulation du mélange visqueux. Le lecteur intéressé pourra se référer aux thèses de Kandhai [55], Latt [56], Malaspinas [14] et Matilas [57] et au livre de Succi [58]. Il est important de mentionner que le développement de la LBM peut être obtenu de différentes manières. En effet, la méthode peut être vue comme une version continue des automates cellulaires ou une version discrétisée de l'équation de Boltzmann. De plus, dans chacune de ces deux approches, il existe plusieurs variantes et les étapes peuvent être effectuées dans un ordre différent.

Sans perte de généralité, il ne sera présenté dans la prochaine section qu'un seul développement, principalement basé sur Malaspinas [14] et Shan [59]. De cette manière, il sera possible de faire apparaitre les paramètres numériques et d'introduire les différentes hypothèses associées à la LBM. Il est important de souligner que le développement de Boltzmann à Navier-Stokes se limitera à un fluide athermal faiblement compressible et que les forces volumiques ne sont pas considérées.

2.1   De Boltzmann à Navier-Stokes

L'idée sous-jacente à la méthode de Boltzmann sur réseau (LBM) est que le comportement macroscopique d'un fluide est indépendant de la nature des particules qui le composent. Ainsi, en définissant des particules fictives dont le comportement peut être facilement simulé, il est possible d'obtenir une approximation de l'écoulement du fluide (voir la citation de Feynman dans [55]).

2.1.1 Équation de Boltzmann sous forme continue

Contrairement aux équations de Navier-Stokes, l'équation de Boltzmann est basée sur une échelle physique différente, l'échelle mésoscopique, qui permet d'étudier le comportement d'un groupe de particules (théorie cinétique des gaz). Si l'on introduit $f(\vec{x}, \vec{e}, t)$ comme étant une probabilité de présence de particules (ou population) au point $\vec{x}$, avec une vitesse $\vec{e}$ et au temps t, son évolution peut être déterminée par l'équation de Boltzmann :

$$(\partial_t + \vec{e}.\nabla)f(\vec{x}, \vec{e}, t) = \Omega \qquad (2.1)$$

avec Ω l'opérateur de collision interparticulaire.

Grâce à ces populations, il est possible de calculer les grandeurs macroscopiques (masse volumique, quantité de mouvement et énergie interne) par intégration dans l'espace des vitesses :

$$\rho(\vec{x}, t) = \int f(\vec{x}, \vec{e}, t)d\vec{e} \qquad (2.2)$$

$$\rho\vec{u}(\vec{x}, t) = \int f(\vec{x}, \vec{e}, t)\vec{e}d\vec{e} \qquad (2.3)$$

$$\rho\varepsilon(\vec{x}, t) = \frac{1}{2}\int f(\vec{x}, \vec{e}, t)(\vec{e} - \vec{u})^2 d\vec{e} \qquad (2.4)$$

Ces grandeurs sont généralement appelées 'moments' et correspondent chacune à un ordre différent en vitesse $\vec{e}$.

Dans le cas d'un gaz monoatomique, on notera que l'énergie interne peut aussi s'exprimer comme $\rho\varepsilon(\vec{x}, t) = 0.5d\rho c_s$ avec d la dimension spatiale du problème et $c_s = \sqrt{RT}$ où T est la température et R la constante des gaz parfaits ($R \approx 8.31\,J.mol^{-1}.K^{-1}$).

Comme l'équation (2.1) est difficile à résoudre à cause de la non linéarité de l'opérateur de collision, Bhatnagar, Gross et Krook (BGK) [60] ont proposé un opérateur de collision simplifié, modélisé par une relaxation vers l'équilibre. L'hypothèse sous-jacente est que la collision entraine les populations vers un état d'équilibre. De cette manière, l'équation (2.1) prend la forme suivante (appelée LBGK) :

$$(\partial_t + \vec{e}.\nabla)f(\vec{x}, \vec{e}, t) = -\frac{1}{\tau}\left(f(\vec{x}, \vec{e}, t) - f^{(eq)}(\vec{x}, \vec{e}, t)\right) \qquad (2.5)$$

avec τ le facteur de relaxation et $f^{(eq)}$ la population d'équilibre. Cette dernière est définie par une fonction de distribution de Maxwell-Boltzmann :

$$f^{(eq)}(\vec{x}, \vec{e}, t) = -\frac{\rho}{(2\pi c_s^2)^{d/2}}exp\left(-\frac{(\vec{u} - \vec{e})^2}{2c_s^2}\right) \qquad (2.6)$$

Par définition, les moments peuvent être indépendamment calculés avec les populations ou les populations d'équilibre :

$$\rho(\vec{x}, t) = \int f(\vec{x}, \vec{e}, t) d\vec{e} = \int f^{(eq)}(\vec{x}, \vec{e}, t) d\vec{e} \tag{2.7}$$

$$\rho \vec{u}(\vec{x}, t) = \int f(\vec{x}, \vec{e}, t) \vec{e} d\vec{e} = \int f^{(eq)}(\vec{x}, \vec{e}, t) \vec{e} d\vec{e} \tag{2.8}$$

$$\rho \varepsilon(\vec{x}, t) = \int f(\vec{x}, \vec{e}, t)(\vec{e} - \vec{u})^2 d\vec{e} = \int f^{(eq)}(\vec{x}, \vec{e}, t)(\vec{e} - \vec{u})^2 d\vec{e} \tag{2.9}$$

En intégrant l'équation LBGK (2.5) sur l'espace des vitesses (voir Annexe A), il est possible d'en déduire les équations de conservations de la masse et de la quantité de mouvement :

$$\partial_t \rho + \nabla.(\rho \vec{u}) = 0 \tag{2.10}$$

$$\partial_t (\rho \vec{u}) + \nabla.(\rho \vec{u} \vec{u}) - \nabla.\boldsymbol{\sigma} = 0 \tag{2.11}$$

avec $\vec{u}\vec{u} = \vec{u} \otimes \vec{u}$, le produit tensoriel du vecteur $\vec{u}$ avec lui-même, et $\boldsymbol{\sigma}$ le tenseur des contraintes calculé comme :

$$\sigma_{\alpha\beta} = -\int f(\vec{x}, \vec{e}, t)(e_\alpha - u_\alpha)(e_\beta - u_\beta) d\vec{e} \tag{2.12}$$

c'est-à-dire que le tenseur est exprimé comme un moment d'ordre 2 en vitesse ($\vec{e}\vec{e}$).

Si cette définition du tenseur assure sa symétrie, elle ne permet pas de fermer le système d'équations (2.10) et (2.11). En effet, il comporte 4 équations pour 10 inconnues (1 masse volumique, 3 vitesses et 6 contraintes).

2.1.2 Équation de fermeture

Afin de fermer le système d'équations (2.10) et (2.11), obtenu à partir de l'équation de Boltzmann, il est nécessaire d'exprimer le tenseur des contraintes à partir des autres grandeurs macroscopiques.

Tout d'abord, il faut appliquer la décomposition de Chapman-Enskog [61, 62] à l'équation LBGK (2.5). Cette décomposition est basée sur une séparation des phénomènes en fonction de

leur échelle de temps (l'advection est plus rapide que la diffusion). Dans cette procédure (voir Annexe B), les populations et les dérivées sont décomposées en plusieurs termes relatifs à chaque échelle de temps. Par exemple, les populations sont exprimées sous la forme suivante :

$$f = f^{(0)} + \epsilon f^{(1)} + \mathcal{O}(\epsilon^2) \tag{2.13}$$

Il est important de noter que le paramètre $\epsilon \ll 1$ est généralement identifié comme étant le nombre de Knudsen ($K_n = l/L$) avec l le libre parcours moyen d'une molécule et L une dimension caractéristique de l'écoulement. Cette étape ajoute donc à la LBM l'hypothèse d'écoulement à faible K_n.

Lorsque la décomposition est appliquée à l'équation LBGK (2.5), il est possible de regrouper les termes par puissance de ϵ :

$$f^{(0)} = f^{(eq)} \qquad \text{Ordre 0} \tag{2.14}$$

$$(\partial_t + \vec{e}.\nabla)f^{(0)} = -\frac{1}{\tau}f^{(1)} \qquad \text{Ordre 1} \tag{2.15}$$

L'équation (2.14) montre que la population $f^{(0)}$ correspond à la fonction d'équilibre. Cela permet de montrer que la décomposition des populations dans l'équation (2.13) revient à séparer les populations entre un terme d'équilibre $f^{(eq)}$ et de non équilibre $\epsilon f^{(1)}$. Cette décomposition sera utilisée ultérieurement dans le document.

Afin de déterminer l'équation de fermeture, l'équation (2.15) est projetée sur une base Hermitienne. L'intérêt de l'utilisation de cette base est double puisque les coefficients de l'expansion des populations peuvent s'exprimer à partir des moments et qu'il existe une relation de récurrence entre les coefficients. Dans le cas d'un fluide athermal faiblement compressible, une troncature à l'ordre 2 de la projection des populations est suffisante pour conserver la masse et la quantité de mouvement. De cette manière, une relation entre les coefficients peut être établie, ce qui permet de relier les grandeurs macroscopiques entre elles. L'équation de fermeture obtenue est alors :

$$\boldsymbol{\sigma} = p\boldsymbol{I} - 2\mu\boldsymbol{S} \tag{2.16}$$

avec p la pression et $\mu = \theta\rho\tau$ où $\theta = k_B T/m$, avec k_B la constante de Boltzmann et m la masse d'une particule.

On notera que l'obtention cette équation nécessite l'introduction de la loi des gaz parfaits sous la forme :

$$p(\vec{x}, t) = \theta\rho(\vec{x}, t) \tag{2.17}$$

La troncature sur $f^{(0)}$ à l'ordre 2 permet de réécrire la fonction d'équilibre $f^{(eq)}$ sous la forme :

$$f^{(eq)}(\vec{x}, \vec{e}, t) = \omega(\vec{e})\rho\left(1 + (\vec{e}.\vec{u}) + (\vec{e}.\vec{u})^2 - \frac{(\vec{u}.\vec{u})}{2}\right) \tag{2.18}$$

avec ω le poids associé à $\vec{e}$.

Cette définition n'est valable que pour un fluide athermal faiblement compressible et ajoute l'hypothèse de petits nombres de Mach ($Ma = |\vec{u}|/c_s$).

2.1.3 Discrétisation en vitesse

L'étape de discrétisation en vitesse est basée sur le principe que les intégrales associées au calcul des coefficients de l'expansion des populations peuvent être exactement évaluées avec une somme pondérée, basée sur une quadrature de Gauss-Hermite. Le choix de cette quadrature est justifié par le fait que le domaine d'intégration est $]-\infty, +\infty[$. Comme les intégrales sont dans l'espace des vitesses, l'application de la quadrature de Gauss-Hermite fait apparaitre des points de Gauss correspondant à des vitesses discrètes $\vec{e}_k$, appelées aussi directions.

Le choix de l'ordre de la quadrature dépend de la troncature sur la population f faite dans la section précédente. Comme précisé auparavant, nous nous sommes limités aux équations de Navier-Stokes pour un fluide athermal faiblement compressible. Dans ce cas, la population f a été tronquée à l'ordre 2, la quadrature de Gauss-Hermite s'applique donc à des polynômes dont l'ordre est au maximum 4 (voir Malaspinas [14] et Shan [59]).

Les moments peuvent ainsi être calculés exactement à partir d'un nombre fini q de populations $f(\vec{x}, \vec{e}_k, t)$. En introduisant la population $f_k(\vec{x}, t)$ de poids ω_k, associée à la direction $\vec{e}_k$, comme :

$$f_k(\vec{x}, t) = \frac{\omega_k}{\omega(\vec{e}_k)} f(\vec{x}, \vec{e}_k, t) \tag{2.19}$$

les moments discrétisés deviennent

$$\rho(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t) \tag{2.20}$$

$$\rho\vec{u}(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t)\vec{e}_k \tag{2.21}$$

et la fonction d'équilibre devient :

$$f_k^{(eq)}(\vec{x}, t) = \omega_k\rho\left(1 + \frac{(\vec{e}_k.\vec{u})}{c_s^2} + \frac{(\vec{e}_k.\vec{u})^2}{2c_s^4} - \frac{\vec{u}^2}{2c_s^2}\right) \tag{2.22}$$

où $c_s = c/\sqrt{3}$, avec c la vitesse de propagation qui sera explicitée dans la section suivante.

De même, dans le tenseur des contraintes, l'expression utilisée pour décrire la viscosité devient :

$$\mu = \rho\tau c_s^2 \tag{2.23}$$

D'un point de vue pratique, la discrétisation de l'espace des vitesses en un ensemble de directions $\{\vec{e}_k\}$ ($k = 0, ..., q-1$) permet de définir les lattices. Cette étape est un point clé de la méthode LBM car elle permet de façonner leur forme, c'est-à-dire la structure de communication de la méthode. Les lattices obtenues sont nommées DdQq, avec d la dimension du problème et q le nombre total de directions. Dans le reste de cette thèse, c'est la lattice D3Q15 [63] qui sera utilisée. En effet, d'après nos tests, lorsqu'elle est comparée aux lattices D3Q19 et D3Q27, elle permet de réduire les temps de calculs tout en conservant une précision similaire. Il est à noter que l'utilisation de la lattice D3Q15 peut générer des effets en damier sur les champs de pression et de vitesse [64]. Si ces effets sont négligeables pour des nombres de Reynolds modérés, il est conseillé d'utiliser les lattices D3Q19 ou D3Q27 pour les écoulements turbulents. L'ensemble associé $\{\vec{e}_k\}$ est défini dans le Tableau 2.1 et est illustré dans la Figure 2.1.

Grâce à cette discrétisation en vitesse, il est maintenant possible d'exprimer l'équation LBGK (2.5) sous la forme :

$$(\partial_t + \vec{e}_k . \nabla) f_k(\vec{x}, t) = -\frac{1}{\tau} \left(f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t) \right) \qquad (2.24)$$

Tableau 2.1: Directions $\vec{e}_k$ et coefficients ω_k pour la lattice D3Q15.

k	0	1	2	3	4	5	6	7	8	9	10	11	12	13
$\vec{x}$	0	c	$-c$	0	0	0	0	c	$-c$	c	$-c$	c	$-c$	c
$\vec{y}$	0	0	0	c	$-c$	0	0	c	$-c$	c	$-c$	$-c$	c	$-c$
$\vec{z}$	0	0	0	0	0	c	$-c$	c	$-c$	$-c$	c	c	$-c$	$-c$
ω_k	2/9	1/9	1/9	1/9	1/9	1/9	1/9	1/72	1/72	1/72	1/72	1/72	1/72	1/72
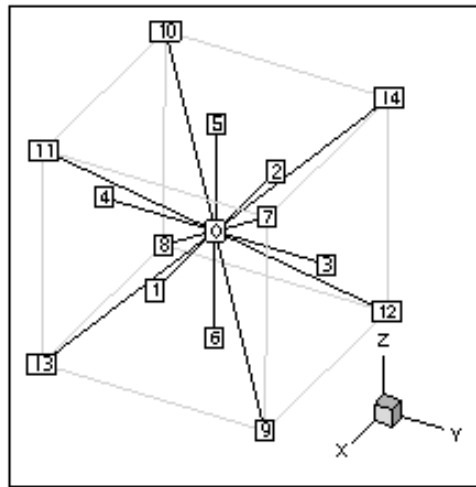
Figure 2.1: Représentation de la lattice D3Q15

2.1.4 Discrétisation spatiale et temporelle

Après avoir effectué la discrétisation de l'espace des vitesses, il faut maintenant discrétiser temporellement l'équation (2.24), c'est-à-dire que l'on introduit le pas de temps δt. On notera que dans le schéma LBM, les populations doivent se déplacer exactement d'une lattice. Autrement dit, $\delta x = c / \delta t$, ce qui définit la discrétisation spatiale. Dans ce cas, le calcul de c_s devient :

$$c_s = \frac{1}{\sqrt{3}} \frac{\delta x}{\delta t} \tag{2.25}$$

L'intégration directe de l'équation (2.24) donne :

$$
\begin{aligned}
f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) &- f_k(\vec{x}, t) \\
&= -\frac{1}{\tau} \int_0^{\delta t} f_k(\vec{x} + \vec{e}_k s, t + s) - f_k^{(eq)}(\vec{x} + \vec{e}_k s, t + s) ds
\end{aligned}
\tag{2.26}
$$

Si on applique la méthode des trapèzes pour calculer l'intégrale, on obtient :

$$
\begin{aligned}
f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) &- f_k(\vec{x}, t) \\
&= -\frac{\delta t}{2\tau} \Big(f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) - f_k^{(eq)}(\vec{x} + \vec{e}_k \delta t, t + \delta t) \\
&\quad + f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t) \Big) + \mathcal{O}(\delta t^2)
\end{aligned}
\tag{2.27}
$$

En introduisant le changement de variable suivant :

$$\tilde{f}_k(\vec{x}, t) = f_k(\vec{x}, t) + \frac{\delta t}{2\tau} \Big(f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t) \Big) \tag{2.28}$$

l'équation (2.27) devient

$$\tilde{f}_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) - \tilde{f}_k(\vec{x}, t) = -\frac{1}{\tilde{\tau}} \Big(\tilde{f}_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t) \Big) \tag{2.29}$$

avec

$$\tilde{\tau} = \frac{\tau}{\delta t} + \frac{1}{2} \tag{2.30}$$

Grâce à ce changement de variable, on obtient une formulation explicite d'ordre 2 en temps. Il est important de noter que le changement de variable affecte la définition de la viscosité. L'équation (2.23) devient :

$$\mu = \rho c_s^2 \delta t \left(\tilde{\tau} - \frac{1}{2} \right) \tag{2.31}$$

Par contre, les calculs de la masse volumique et de la vitesse ne sont pas affectés. Dans le cas plus général où une force volumique est considérée, le changement de variable entraine l'introduction de cette force dans le calcul des vitesses [14, 65]. Dans le reste de la thèse, le tilde (~) sera omis par mesure de simplicité et seules les populations avec changement de variable seront considérées.

2.2 Équation de collision-propagation

Commençons par résumer le schéma LBM présenté dans la section 2.1. L'équation LBGK discrétisée prend la forme :

$$f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) - f_k(\vec{x}, t) = -\frac{1}{\tau} \left(f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t) \right) \tag{2.32}$$

avec la fonction d'équilibre définie comme :

$$f_k^{(eq)}(\vec{x}, t) = \omega_k \rho \left(1 + \frac{(\vec{e}_k . \vec{u})}{c_s^2} + \frac{(\vec{e}_k . \vec{u})^2}{2c_s^4} - \frac{\vec{u}^2}{2c_s^2} \right) \tag{2.33}$$

où les poids ω_k dépendent de la lattice utilisée et la vitesse du son c_s est définie comme :

$$c_s = \frac{1}{\sqrt{3}} \frac{\delta x}{\delta t} \tag{2.34}$$

Dans chaque lattice, une masse volumique et un vecteur vitesse peuvent être calculés directement à partir des populations :

$$\rho(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t) \tag{2.35}$$

$$\vec{u}(\vec{x}, t) = \frac{1}{\rho(\vec{x}, t)} \sum_{k=0}^{q-1} f_k(\vec{x}, t) \vec{e}_k \tag{2.36}$$

Le paramètre de relaxation τ est relié à la viscosité par la relation suivante :

$$\tau = \frac{\mu}{\rho c_s^2 \delta t} + \frac{1}{2} \tag{2.37}$$

Dans la section 2.1, nous avons montré que la LBM permet d'obtenir une solution des équations de Navier-Stokes incompressibles et athermales, sous contrainte de faible nombre de Mach et de Knudsen. Dans le cadre de la LBM, ces deux nombres s'expriment comme :

$$M_a = \frac{|\vec{u}|}{c_s} \tag{2.38}$$

$$K_n = \frac{\mu}{\rho L c_s} \tag{2.39}$$

avec L une dimension caractéristique du problème étudié.

Afin de déterminer l'ordre de convergence spatiale, il est nécessaire d'appliquer une analyse asymptotique de l'équation de lattice Boltzmann [66, 67]. Ainsi, en utilisant l'échelle diffusive (i.e. $\delta t \propto \delta x^2$), on montre que la LBM permet d'obtenir une solution des équations de Navier-Stokes (vitesse et pression) avec une précision d'ordre 2 en espace sur la vitesse. L'utilisation de l'échelle diffusive ($\delta t \propto \delta x^2$) entraine une précision en temps d'ordre 1. D'un point de vue pratique, lorsque l'on cherche à vérifier l'ordre de convergence spatiale, l'utilisation de l'échelle diffusive implique de conserver une valeur fixe du facteur de relaxation τ, ce qui permet de garder un ratio $\delta t/\delta x^2$ constant. Il est important de souligner que les développements mathématiques associés à l'étude de la convergence se limitent généralement à des domaines périodiques. Pour d'autres configurations, comme des conditions aux limites de Dirichlet en vitesse, la convergence spatiale est largement affectée [67].

Il est aussi intéressant de regarder plus précisément les calculs associés à la LBM. Il est possible de réécrire l'équation (2.32) sous la forme suivante :

$$f_k^+(\vec{x}, t) = f_k(\vec{x}, t) - \frac{1}{\tau}\Big(f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t)\Big) \tag{2.40}$$

$$f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) = f_k^+(\vec{x}, t) \tag{2.41}$$

l'équation (2.40) correspond à l'étape de collision et l'équation (2.41) à celle de propagation. On remarque alors que les calculs nécessaires à l'application du schéma LBM, c'est-à-dire les équations (2.40), (2.33), (2.35) et (2.36), sont simples et locaux. La localité signifie que les calculs associés à une lattice ne nécessitent pas d'autres informations que celles présentes dans la lattice. La seule étape nécessitant un transfert de l'information étant l'étape de propagation, définie par l'équation (2.41). On remarque alors que le transfert d'informations est structuré par les directions $\vec{e}_k$. Toutes ces propriétés donnent à la LBM une très bonne efficacité pour le calcul parallèle. Il est important de souligner que ces avantages ne sont pas tous intrinsèquement reliés à la LBM, mais pourraient s'appliquer à d'autres schémas utilisant un maillage structuré cartésien. Les avantages intrinsèques de la LBM sont plutôt reliés à l'intégration simple de modèles de phénomènes physiques dont l'origine est microscopique. Par exemple, on peut citer l'intégration des modèles rhéologiques [16, 54, 55] ou la modélisation de l'interaction entre les phases pour les écoulements polyphasiques [68-70]. L'intégration de la rhéologie sera traitée plus en détail dans la section 2.5.

2.3 Définition des conditions aux limites

Les conditions aux limites servent à contraindre la solution numérique sur les frontières du domaine de simulation. En effet, pour pouvoir simuler un écoulement donné, les conditions aux limites doivent modéliser les phénomènes physiques qui apparaissent aux différentes surfaces du volume occupé par le fluide. Les exemples les plus courants de tels phénomènes sont les surfaces libres, l'attachement des fluides à une paroi solide et les profils d'entrée et de sortie dans les canaux. Puisque l'échelle physique des écoulements simulés est macroscopique, il est nécessaire d'imposer des conditions aux limites macroscopiques sur les frontières du domaine. Comme nous l'avons vu dans la section 2.1, contrairement aux méthodes qui résolvent directement les équation de Navier-Stokes, la LBM utilise une variable primaire mésoscopique (une population de particules f_k), ce qui complique largement l'imposition d'une contrainte macroscopique. En effet, s'il est très simple de calculer la masse volumique et la vitesse à partir des populations, comme défini dans les équations (2.35) et (2.36), le calcul inverse n'a pas de solution unique. Ceci explique pourquoi les conditions aux limites sont une difficulté intrinsèque à la LBM et requièrent un changement de paradigme par rapport aux méthodes classiques de la CFD. Le but

de cette section est de donner un aperçu des stratégies d'imposition de vitesses non nulles sur des frontières courbes, des explications plus détaillées se trouvant dans l'article 1 (section 4.2).

2.3.1 La règle du rebond

Afin d'imposer une vitesse nulle sur une frontière, l'approche la plus couramment utilisée est celle de la règle du rebond « bounce-back rule » [71, 72], qui permet de définir les populations manquantes comme :

$$f_{k'}(\vec{x}, t + \delta t) = f_k^+(\vec{x}, t) \tag{2.42}$$

avec k' la direction opposée à k et f_k^+ la population post-collision définie par l'équation (2.40).
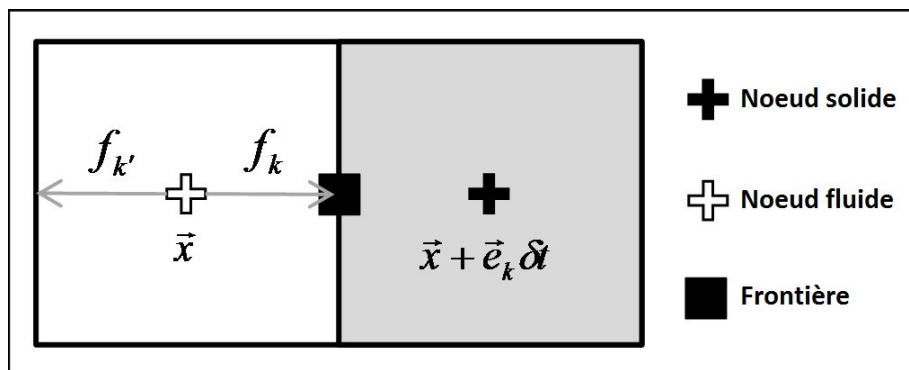
Figure 2.2: Illustration de la règle du rebond (tirée de l'article 1)

Comme illustrée dans la Figure 2.2, la population $f_k^+(\vec{x}, t)$ qui devrait être perdue (car propagée vers une zone solide ou en dehors du domaine) est utilisée pour calculer la direction opposée. Cette stratégie peut être étendue à l'imposition de vitesse non nulles [72] de la manière suivante :

$$f_{k'}(\vec{x}, t + \delta t) = f_k^+(\vec{x}, t) - 2\omega_k \rho \frac{\vec{e}_k \cdot \vec{u}_b}{c_s^2} \tag{2.43}$$

avec $\vec{u}_b$ la vitesse de l'obstacle à la frontière.

Il est important de souligner que la position de la frontière est toujours considérée comme étant située à $\vec{x} + \vec{e}_k \delta t/2$, c'est-à-dire au bord de la lattice fluide. Lorsqu'appliquée à mur droit positionné exactement aux bords des lattices, cette approche permet de conserver l'ordre de précision de la LBM en vitesse. Dans le cas plus général d'une frontière courbe, son utilisation entraine une perte de précision et une réduction de l'ordre de convergence [67, 73, 74].

Afin de réduire la perte de précision associée à l'imposition d'une vitesse non nulle sur une frontière courbe, de nombreux travaux de recherche ont proposé des solutions basées sur des approches différentes. Par mesure de simplicité, nous n'introduirons que les solutions facilement applicables à une géométrie 3D complexe, c'est-à-dire les méthodes basées sur l'interpolation ou l'extrapolation en fonction de la distance à la frontière [75-79] et les conditions aux limites immergées [80-83].

2.3.2 Stratégies d'interpolation ou d'extrapolation

L'idée principale de ce type de stratégie de conditions aux limites est d'utiliser la distance à la frontière pour augmenter la précision. Comme illustré dans la Figure 2.3, pour chaque duo de lattices fluide-solide, la fraction Δ (appelée distance) est utilisée pour décrire exactement la position de la frontière.
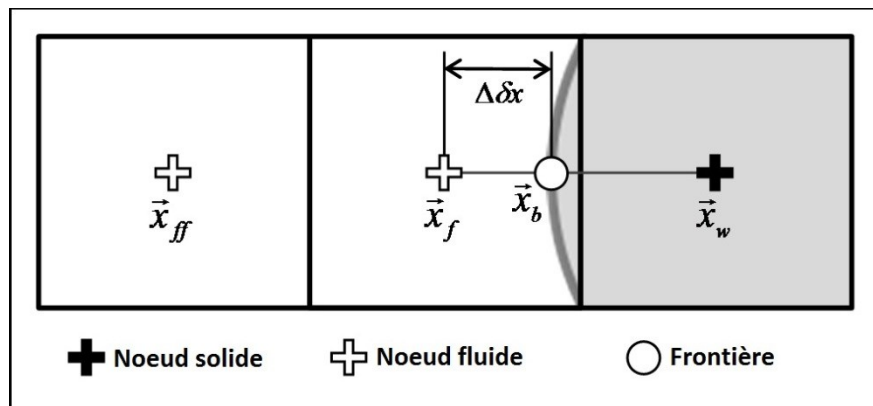
Figure 2.3: Illustration de la distance à la frontière (tirée de l'article 1)

La différence entre les méthodes se trouve dans la manière d'utiliser les distances Δ pour améliorer la précision. Par exemple, la méthode d'extrapolation « extrapolation method » EM [78] l'utilise pour calculer des populations d'équilibre et de non équilibre fictives au nœud solide $\vec{x}_w$. Pour ce faire, la fonction d'équilibre est calculée avec une vitesse et une masse volumique extrapolées à partir des nœuds voisins en $\vec{x}_f$ et $\vec{x}_{ff}$, la partie de non équilibre étant directement extrapolée à partir des voisins (voir l'article 1 pour le détail des calculs). La définition des populations de non équilibre est basée sur la décomposition présentée dans l'équation (2.13) et réécrite de la manière suivante :

$$f_k^{(neq)}(\vec{x}, t) = f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t) \tag{2.44}$$

Une autre approche, proposée par Bouzidi, Firdaouss et Lallemand [77], interpole les populations manquantes à l'aide des populations de post-collision voisines. Ainsi, les populations sont calculées comme :

$$f_{k'}(\vec{x}, t + \delta t) = 2\Delta f_k^+(\vec{x}, t) + (1 - 2\Delta)f_k^+(\vec{x} - \vec{e}_k\delta t, t) + 2\omega_k\rho\frac{\vec{e}_k.\vec{u}_b}{c_s^2} \quad si\ \Delta < 0.5 \tag{2.45}$$

$$f_{k'}(\vec{x}, t + \delta t) = \frac{1}{2\Delta}f_k^+(\vec{x}, t) + \frac{(2\Delta - 1)}{2\Delta}f_k^+(\vec{x} - \vec{e}_k\delta t, t) + \frac{1}{\Delta}\omega_k\rho\frac{\vec{e}_k.\vec{u}_b}{c_s^2} \quad si\ \Delta \geq 0.5 \tag{2.46}$$

Ces méthodes permettent une augmentation significative de la précision et une conservation de l'ordre de convergence en vitesse de la LBM [74, 78, 84]. Cependant, il y a deux désavantages qui sont la perte de la localité des calculs (utilisation des lattices voisines) et la difficulté de calculer les distances dans le cas d'une géométrie complexe, comme une pale ou un milieu poreux.

2.3.3 Conditions aux limites immergées

Historiquement développées pour les méthodes d'éléments et de volumes finis, les conditions aux limites immergées (IBM) [10, 40, 85] utilisent des points de contrôle pour contraindre la vitesse du fluide environnant. Comme illustré dans la Figure 2.4, en immergeant un ensemble de points décrivant la forme d'un obstacle, il est possible de contraindre le fluide à avoir sa vitesse, sans définir de frontière au domaine fluide. Ce type d'approche est très largement utilisé dans le cas d'obstacles mobiles puisqu'il permet de ne pas avoir à rediscrétiser le volume fluide en fonction du déplacement d'un objet.

Plusieurs adaptations ont été proposées pour la LBM [80-83] et sont basées sur deux étapes : une interpolation pour calculer la différence entre la vitesse aux points de contrôle et la celle de l'obstacle; puis une distribution de la correction aux lattices voisines à l'aide d'une force volumique. La différence entre les méthodes se trouve dans la manière de redistribuer la correction. Par exemple la IB-LBM [83] propose de corriger la vitesse en deux étapes, d'abord dans le calcul des vitesses puis dans l'ajout d'une force volumique. Cette approche est basée sur

la définition de la force volumique proposée par Guo *et al*. [65] et couple l'ensemble des corrections à l'aide d'un système matriciel (voir l'article 1 pour le détail des calculs).
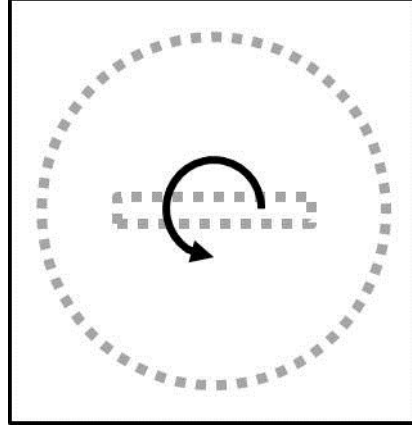
Figure 2.4: Illustration d'une condition aux limites immergée

La technique de forçage « forcing technique », proposée par Derksen *et al*. [86], est basée sur une correction temporelle de la force volumique $\vec{g}_j^{(t)}$ définie comme :

$$\vec{g}_j^{(t)} = \alpha \vec{g}_j^{(t-1)} + \beta \vec{u}_j^{(t)} \tag{2.47}$$

avec α et β des paramètres numériques déterminés empiriquement et $\vec{u}_j^{(t)}$ la vitesse interpolée au point de contrôle j de coordonnées $x_j^{(t)}$.

La fonction d'interpolation G est utilisée pour le calcul des vitesses aux points de contrôle

$$\vec{u}_j^{(t)} = \sum_i G\left(x_j^{(t)}\right) \vec{u}(\vec{x}_i, t) \tag{2.48}$$

avec $\vec{u}(\vec{x}_i, t)$ les vitesses dans les i lattices environnantes.

La redistribution des corrections $\vec{g}_j^{(t)}$ sur les lattices environnantes utilise aussi la fonction d'interpolation G :

$$\vec{g}(\vec{x}_i, t) = \sum_j G\left(x_j^{(t)}\right) \vec{g}_j^{(t)} \tag{2.49}$$

Ces méthodes permettent donc de ne pas rediscrétiser le domaine en fonction du déplacement d'un objet et de ne pas avoir à initialiser de nouvelles lattices fluides.

2.4 Mouvement d'une partie mobile

Lorsque le problème simulé comporte des objets mobiles, il est nécessaire de modéliser l'action de leurs déplacements sur le fluide. Dans le cas des conditions aux limites immergées, ce traitement est largement simplifié puisqu'il se limite à déplacer les points de contrôle. À l'inverse, pour les autres stratégies de conditions aux limites (règle du rebond et méthodes d'interpolation ou d'extrapolation), il est nécessaire de refaire la discrétisation en fonction du déplacement des objets. Comme la LBM est appliquée à des maillages cartésiens structurés, l'étape de discrétisation se limite à déterminer l'ensemble des nœuds situés à l'intérieur des parties solides. Il est important de souligner que cette étape ne comporte pas de difficulté majeure, même dans le cas de géométries complexes. À l'inverse, l'initialisation des lattices nouvellement fluides, illustrée dans la Figure 2.5, est une difficulté intrinsèque à la méthode. En effet, de la même manière qu'il est difficile d'imposer une condition aux limites macroscopique, les initialisations souffrent de la nature mésoscopique des populations.
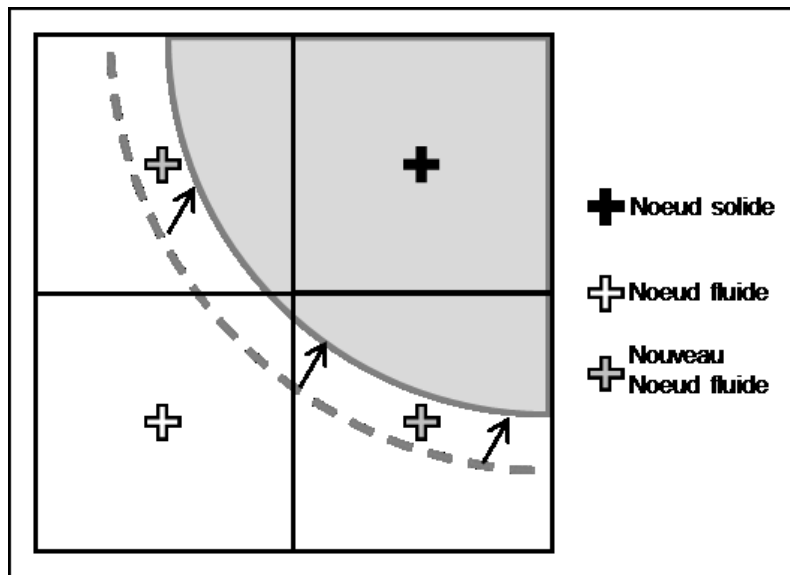
Figure 2.5: Illustration de nouvelles lattices fluides après mouvement d'un objet

Afin de déterminer les populations des lattices nouvellement fluides, plusieurs façons sont envisageables. Par exemple, il est possible d'interpoler les vitesses et les masses volumiques des lattices voisines, puis de les injecter dans la fonction d'équilibre définie par l'équation (2.33). De

même, il est possible d'interpoler directement les populations voisines. Ces différentes approches ont un niveau de précision équivalent, comme rapporté dans [87], mais présentent le désavantage de générer des oscillations en vitesse et en masse volumique autours des objets mobiles [88]. Afin de réduire ces oscillations, il est préférable d'utiliser une initialisation avec un terme correctif basé sur les populations de non équilibre « non-equilibrium corrected refill » [88].

Cette approche nécessite d'abord de choisir une direction d'extrapolation $\vec{e}_i^{(ex)}$, qui est ensuite utilisée pour déterminer une vitesse $\tilde{u}$ et une masse volumique $\tilde{\rho}$ extrapolées. À partir de ces données, les populations sont calculées comme :

$$f_k(\vec{x}, t) = \tilde{f}_k^{(eq)}(\tilde{u}, \tilde{\rho}) + f_k^{(neq)}\left(\vec{x} + \vec{e}_i^{(ex)}\delta t, t\right) \tag{2.50}$$

Ainsi, l'initialisation des nouvelles populations est corrigée avec les populations de non équilibre des lattices voisines. Cette correction permet de réduire largement les oscillations et d'améliorer le champ de vitesse autour de l'obstacle [88]. Il est important de souligner que l'étape de sélection de la direction d'extrapolation $\vec{e}_i^{(ex)}$ n'est pas générique. En effet, il n'existe pas de formule pour calculer cette direction et sa détermination est laissée à la discrétion de l'utilisateur.

2.5 Intégration des modèles rhéologiques

Comme nous l'avons vu dans la section 1.2.2, l'expression du tenseur des contraintes, dans le cas de modèles non newtoniens sans effet d'élasticité, prend la forme suivante :

$$\boldsymbol{\sigma} = p\boldsymbol{I} - 2\eta(\dot{\gamma})\boldsymbol{S} \tag{2.51}$$

Dans ce cas, la viscosité η est fonction du taux de cisaillement $\dot{\gamma} = \sqrt{2\boldsymbol{S}:\boldsymbol{S}}$ ce qui implique que sa valeur n'est plus constante dans le temps et dans l'espace. La dépendance de la viscosité en fonction du taux de cisaillement est définie par le modèle rhéologique utilisé. Afin d'intégrer ce modèle dans le schéma LBM, il suffit de modifier le calcul du facteur de relaxation. Son expression devient alors :

$$\tau(\dot{\gamma}) = \frac{\eta(\dot{\gamma})}{\rho c_s^2 \delta t} + \frac{1}{2} \tag{2.52}$$

avec η calculé grâce l'équation du modèle.

Il est important de noter que cette modification n'altère en rien le développement présenté dans la section 2.1, c'est-à-dire que toutes les propriétés de la méthode LBM sont conservées. Afin de conserver la localité complète de la phase de collision, le calcul du tenseur du taux de déformation $\boldsymbol{S}$ n'est pas calculé à partir des vitesses des lattices voisines. En effet, il est possible d'utiliser une expression différente du tenseur $\boldsymbol{S}$ [62, 89] basée sur les populations :

$$S_{ij} = -\frac{1}{2\tau\rho c_s^2 \delta t} \sum_k \left(\vec{e}_{ki}\vec{e}_{kj} - \frac{\delta_{ij}}{D}\vec{e}_k.\vec{e}_k \right) f_k^{(neq)} \qquad (2.53)$$

Cependant, comme dans l'équation (2.53) $\boldsymbol{S}$ dépend de τ, l'équation (2.52) devient implicite. Ainsi, la détermination de τ devrait être réalisée à l'aide d'une méthode de Newton-Raphson ou de point fixe. Comme cette étape doit être appliquée dans chaque lattice et à chaque itération, le coût en temps de calcul peut devenir prohibitif. Le calcul du facteur de relaxation τ est donc généralement traité avec une approche explicite, c'est-à-dire que la valeur utilisée dans l'équation (2.53) est celle au pas de temps précédent [14, 90]. De cette manière le traitement de la rhéologie se fait facilement avec la LBM.

Par rapport à une simulation LBM newtonienne, l'intégration d'un modèle rhéologique complique la procédure de simulation. En effet, comme la variation totale de viscosité est représentée par une variation du facteur de relaxation τ, celui-ci doit rester dans une plage qui conserve la convergence du schéma. D'après nos tests, cette plage se trouve entre $0.5 + eps$ et 4, la valeur de eps étant dépendante du problème simulé. Par exemple, dans le cas d'un modèle rhéofluidifiant (ou pseudo-plastique), il est nécessaire de choisir une valeur de $\tau(\dot{\gamma} = 0)$, à taux de cisaillement nul, assez grande pour que la valeur du facteur de relaxation à taux de cisaillement maximal $\tau(\dot{\gamma} = \dot{\gamma}_{max})$ n'entraine pas la divergence du schéma. En pratique, cette condition limite la vitesse maximale simulable au travers du nombre de Mach, défini par l'équation (2.38). En effet, comme $\delta t \propto \tau$, une augmentation du facteur de relaxation réduit la vitesse de lattice $c_s = \delta x / \sqrt{3}\delta t$. Comme il est nécessaire de conserver un nombre de Mach faible ($Ma = |\vec{u}|/c_s$), cela peut réduire drastiquement la vitesse maximale $|\vec{u}|$ pour laquelle la solution à un sens.

Plusieurs modèles rhéologiques ont ainsi été appliqués avec succès dans la LBM. Pour les modèles sans viscoélasticité, on notera l'utilisation de modèles de loi de puissance [15, 16], de

Carreau-Yasuda [17, 18], de Bingham [27, 90] et de Casson [17, 90]. Il est important de mentionner que dans le cas des modèles viscoélastiques, il est nécessaire d'ajouter une équation supplémentaire afin de transporter les termes du tenseur de conformation [14, 91].

2.6   La LBM appliquée aux cuves agitées

Dans le cas de la méthode de Boltzmann sur réseau, ce sont principalement des turbines Rushton qui ont été simulées en régime turbulent. La géométrie est modélisée à l'aide de la technique de forçage [86] présentée à la section 2.3.3 et la turbulence est simulée directement (DNS) ou traitée grâce à un modèle de simulation aux grandes échelles « Large Eddy Simulation (LES) » [86], suivant les nombres de Reynolds atteints. Les simulations newtoniennes [86, 92, 93] ont permis de valider l'utilisation de la LES dans ce contexte, par comparaison avec des données expérimentales, des résultats de simulations numériques directes (DNS) et d'équations de Reynolds moyennées (RANS). Dans le cas non newtonien, la simulation d'un liquide thixotropique [54, 94] a permis d'étudier l'impact du nombre de Deborah sur la forme de l'écoulement. On notera aussi la simulation du mélange de deux liquides avec des masses volumiques et des viscosités différentes, à l'aide d'une méthode de type 1-fluide [95, 96].

Dans le cas des suspensions solide-liquide, l'utilisation d'une approche de type particules discrètes (ou Euler-Lagrange) [26] a permis l'étude des temps de séjour [97] et de la dissolution des particules [98]. L'impact de la rhéologie sur l'évolution de la suspension a aussi été étudié pour des liquides de Bingham [27]. Cette approche de simulation Euler-Lagrange a aussi été étendue à la simulation de suspensions gaz-liquide [99, 100]. Il est à noter qu'un autre groupe de recherche a appliqué une méthode de Boltzmann sur réseau avec des particules colorées (c'est-à-dire avec l'ajout d'une équation de transport d'une concentration) afin d'étudier le mélange d'un système simplifié [101].

À partir de cette revue de littérature, il ressort que la LBM est une méthode efficace pour la simulation du mélange turbulent. Autrement dit, lorsqu'elle est couplée à un modèle LES, elle permet de reproduire globalement la création et le transport des tourbillons au sein d'un mélangeur industriel. Dans le cas du mélange visqueux, ce sont les interactions entre la pale raclante et la cuve ainsi que la forme de la pale qui génèrent le mélange dispersif et distributif. Aussi, le traitement de la géométrie et l'imposition des conditions aux limites doivent être assez précis pour prédire correctement les performances du système de mélange.

CHAPITRE 3   ORGANISATION DE LA THÈSE

La simulation des écoulements visqueux en cuves agitées requiert un traitement précis de la géométrie, de la modélisation de l'impact des parties mobiles sur le fluide et de l'intégration des modèles rhéologiques. Dans ce cas, l'utilisation des méthodes classiques de la CFD entraine généralement un compromis entre la précision et les temps de calcul, limitant ainsi les possibilités de simulation d'écoulements polyphasiques ou à rhéologies complexes. À l'inverse, la méthode de Boltzmann sur réseau (LBM) permet un traitement simplifié des géométries complexes et une intégration naturelle des modèles rhéologiques sans effet d'élasticité. Cependant, la définition des conditions aux limites et le traitement de parties mobiles n'étant pas triviaux, il est nécessaire de déterminer les erreurs qui peuvent être générées par ces deux aspects. Finalement, comme l'intégration des modèles rhéologiques est simplifiée, il est intéressant d'étudier les limites atteignables en termes de complexité.

Afin d'atteindre l'objectif principal, les objectifs spécifiques sont :

- Comparer les différentes stratégies pour l'imposition des conditions aux limites en LBM;

- Déterminer la précision de la LBM pour des écoulements visqueux dans des géométries complexes;

- Caractériser l'applicabilité de la LBM pour des rhéologies complexes sans effets d'élasticité.

Afin de déterminer la stratégie la plus appropriée, l'article 1 présente une comparaison de trois stratégies de conditions aux limites couramment utilisées dans la littérature et facilement applicables à des géométries complexes 3D. D'abord, leurs impacts sur la précision de la LBM sont quantifiés à l'aide de la simulation de l'écoulement de Couette cylindrique. Cette étape permet aussi l'étude des paramètres numériques associés à chaque stratégie. La comparaison est ensuite étendue à la simulation de deux systèmes de mélange utilisant une ancre et un Paravisc. À l'aide d'un repère Lagrangien basé sur la pale, les trois stratégies de conditions aux limites sont comparées sur la qualité de prédiction de la consommation de puissance et de la capacité de

pompage. Les impacts des trois stratégies sur l'efficacité de la LBM pour le calcul parallèle sont aussi quantifiés.

L'article 2 s'intéresse à la précision de la méthode de Boltzmann sur réseau dans le cas de géométries complexes. Afin de maximiser la précision, seule la stratégie de conditions aux limites basée sur l'extrapolation est utilisée. Tout d'abord, la simulation de l'écoulement de Couette cylindrique permet d'étudier la sensibilité de la méthode à des modifications mineures sur les frontières du domaine de simulation. Ensuite, l'écoulement au sein du système de mélange Maxblend est simulé pour différentes configurations. Les prédictions de consommations de puissance et de capacités de pompage sont comparées avec les données expérimentales et numériques disponibles dans la littérature. Premièrement, à l'aide d'un repère Lagrangien basé sur la pale, l'impact du dégagement au fond de la cuve est caractérisé. Deuxièmement, la simulation de la configuration avec contre-pales, nécessitant l'utilisation du repère naturel, permet d'étudier la précision de la méthode dans le cas d'une pale en rotation (c'est-à-dire avec une partie mobile).

Le dernier article traite de l'impact de la rhéologie sur les mécanismes associés à la création du pompage dans le système de mélange Maxblend. D'abord, dans le cas newtonien, l'évolution de la capacité de pompage en fonction du régime d'écoulement est comparée avec les données expérimentales et numériques disponibles dans la littérature. Cette étape permet d'étudier la transformation de l'écoulement secondaire (composantes radiales et axiales) dans le régime laminaire profond. L'étude est ensuite étendue à la simulation d'un liquide fortement rhéofluidifiant (indice de puissance de 0.05) à l'aide d'un modèle de Carreau-Yasuda. De cette manière, l'impact de la rhéologie sur la transformation de l'écoulement secondaire est caractérisé. Cette étape permet aussi de déterminer les limitations associées à l'utilisation de la LBM dans le cas de rhéologies complexes (fortement rhéofluidifiantes dans ce cas).

Les contributions scientifiques associées à ce travail sont :

- Une comparaison de stratégies pour l'imposition des conditions aux limites dans le cas de géométries complexes;

- Une étude de la précision de la LBM pour la simulation de la rotation d'un objet de forme complexe;

- La simulation de l'agitation d'un liquide fortement rhéofluidifiant (indice de puissance de 0.05).

Ce travail a nécessité de développement complet d'un code LBM tridimensionnel dont les calculs peuvent être effectués sur un grand nombre de processeurs. Les particularités du code sont relatives à sa capacité à définir des conditions aux limites sur des géométries complexes ainsi qu'à prendre en compte la rotation des objects. Il est à noter que les résultats présentés dans l'article 1 ont été obtenus grâce à un code LBM développé par D. Vidal.

CHAPITRE 4   COMPARAISON DES DIFFÉRENTES STRATÉGIES POUR L'IMPOSITION DES CONDITIONS AUX LIMITES EN LBM

4.1   Présentation du premier article

Auteurs : Vincent Stobiac, Philippe Tanguy, François Bertrand.

Dans cet article, trois stratégies d'imposition de conditions aux limites sont comparées dans le cadre de la simulation d'écoulements visqueux en cuves agitées. Les stratégies ont été sélectionnées parmi les approches les plus couramment utilisées dans la littérature : la méthode du rebond modifié (MBB), la méthode d'extrapolation (EM) et la méthode de conditions aux limites immergées (IB-LBM), chacune de ces stratégies étant représentative d'une classe de conditions aux limites possédant des propriétés similaires. Tout d'abord, l'écoulement de Couette cylindrique a été simulé afin de vérifier l'impact des trois stratégies sur l'ordre de convergence du schéma LBM. Il ressort que seule la méthode d'extrapolation est capable de conserver la précision du deuxième ordre pour la convergence spatiale de la vitesse. Ensuite, à l'aide d'un code LBM massivement parallèle, les simulations sont étendues au cas des écoulements dans des mélangeurs raclants (ancre et Paravisc). Le traitement de la géométrie est simplifié par l'utilisation d'un repère Lagrangien fixe par rapport à la pale. Ainsi, les trois stratégies sont comparées sur la convergence spatiale des prédictions de consommation de puissance et de capacité de pompage. Si tous les résultats LBM sont globalement en accord avec les données expérimentales et numériques disponibles dans la littérature, il ressort que la condition aux limites immergées semble moins adaptée aux mélangeurs raclants. À l'inverse, la méthode du rebond modifié, malgré sa simplicité, permet d'obtenir des prédictions équivalentes à celles de la méthode d'extrapolation. Finalement, l'impact des trois stratégies sur les performances en calcul parallèle est aussi quantifié. Cela montre que seule la stratégie basée sur une condition aux limites immergées perturbe les propriétés de la méthode de Boltzmann sur réseau.

Note : Dans cet article, le terme « Lagrangian frame of reference » réfère à un repère tournant fixé sur la pale.

4.2 Boundary conditions for the lattice Boltzmann method in the case of viscous mixing flows

4.2.1 Summary

This paper examines the performance of different boundary condition strategies for the lattice Boltzmann simulation of industrial viscous mixing flows. Three different strategies were chosen from the most popular approaches, which are the staircase approaches (bounce-back rules), the extrapolation or interpolation methods, and the immersed boundary methods. First, the order of convergence of the selected methods to impose boundary conditions is verified on the 3D Couette flow. This work clearly shows that only the extrapolation method is capable of preserving the second order accuracy of the lattice Boltzmann method. Second, a highly parallel LBM scheme is used to simulate fluid flow with close-clearance mixing systems in the Lagrangian frame of reference. The convergence rates obtained with the different boundary condition strategies are compared on the basis of two characteristic mixing numbers, the power number and the pumping rate. The results agree well with experimental data and finite element simulation results, and surprisingly enough, the modified bounce back rule provides a reliable accuracy despite its simplicity. Finally, the impact of the boundary condition strategies on the workload balance and the memory usage is analyzed. It appears that only the immersed boundary condition strategy modifies the parallel efficiency of the lattice Boltzmann method, yet no significant effect is observed on the memory usage.

4.2.2 Introduction

Mixing of fluids in stirred tanks is a common activity in many industries such as chemical, pharmaceutical and food processing. During the batch process, the mixing is driven by impellers which are chosen relative to the process characteristics and the fluid properties. Given that there are a large number of important parameters to control the mixing efficiency (bottom clearance, number and position of impellers, speed ratio, etc), its optimisation is a difficult task not to mention costly on an experimental level. In order to reduce this cost, computational fluid dynamics (CFD) has been largely used to compare the performance of mixing systems [41, 43, 45] and to optimize mixing configuration [36, 42, 46, 52, 102, 103]. Another distinguished advantage of CFD is its capacity to access physical variables (velocity, density and shear stress,

etc) inside a system without disturbing the flow. In addition, the simulated flow field can be used to compute characteristic macroscopic values such as mixing time [36, 41, 46, 103], power consumption [12, 13, 36, 41, 42, 44, 46, 48, 51, 52, 103-105] and pumping capacity [13, 41, 46, 106].

One key aspect of the simulation process is the modeling of the action of impellers on the flow, which requires the imposition of a velocity profile along moving surfaces. This task is complicated due to the unfeasibility of remeshing after each time step. Thus, what is required for a fixed discretization is a technique capable of imposing different velocity profiles at different places. Several solutions with entirely different approaches have been proposed in the literature. The sliding mesh (SM) technique widely used with baffled vessels decomposes the domain into two coaxial subdomains, one in the impeller region and its complementary which extends to the tank wall and contains the baffles. This technique is limited to impeller motions based on one single axis and requires communication between the different parts. In order to describe more complex motions, i.e. rotations around several axes, the classes of fictitious domain methods [10] and immersed boundary methods [9] consider a fully fluid domain in which the fluid velocity is constrained at various control points representing the immersed solid parts. Finally, for fully periodic flow, the steady state solution can be computed by employing the Lagrangian frame of reference [37]. In this case, impellers are considered to be fixed and then simply defined by a homogeneous Dirichlet (i.e. zero velocity) boundary condition. This approach is limited to configurations without baffles and with impellers positioned along the same axis, with the same velocity. For the particular case of viscous mixing, no baffles are generally required so that this approach can generally be used, which greatly simplifies the simulation process. For this reason, this strategy was chosen in this work.

Although different CFD methods have been applied to simulate hydrodynamics in stirred tanks, the finite element method (FEM) appears to be the most popular approach for the laminar and transition regimes, as a lot of mixing configurations have been simulated. Using the Lagrangian frame of reference, the hydrodynamics of the Paravisc impeller [41], double helical ribbons (DHR) [12, 37, 43], the Maxblend impeller (without baffles) [13, 36, 43, 44], dough mixers [42] and the Rushton turbine (without baffles) [107] have been analysed. These simulations have allowed to quantify the mixing of Newtonian [12, 13, 36, 37, 41-44, 107] and non-Newtonian flows [12, 13, 41, 42], the power consumption [12, 13, 36, 41, 42, 44], the pumping capacity [13,

41] and the mixing time [36, 41] in specific mixing systems. For planetary mixers, the use of the Lagrangian frame of reference is no longer possible and more complex boundary condition strategies are required, as explained in the previous paragraph. For instance, a three-blade planetary mixer has been simulated [44] using the so-called virtual finite element method (VFEM) [40], which belongs to the category of fictitious domain methods. In the same manner, a two blade planetary mixer has been simulated [45] by a simplified version of the VFEM, implemented in FIDAP (ANSYS). For the simulation of a planetary pin mixer [108], another type of fictitious domain method, called the mesh superposition technique (MST) [109], has been applied. In order to simulate baffled mixing configurations or to access unsteady behaviour, the same techniques have been applied. For instance, the VFEM has been used for the Maxblend impeller (baffled and unbaffled) [13, 36, 44] as well as for coaxial mixers comprised of an anchor and a Rushton turbine [103] or a system of rods [105]. For the Superblend [46], comprised of a Maxblend and a DHR impeller, the SM technique was employed for the Maxblend, coupled with the VFEM for the DHR.

As for mixing flows in turbulent regime, a lot of simulations have been performed with the finite volume method (FVM) in the case of tanks with Rushton turbines [48-51]. The action of the impeller on the fluid is generally achieved by the SM technique or by similar approaches such as the multiple reference frames (MRF) method, which can be viewed as a simplified version of the SM technique only valid for steady-state flows. These simulations have permitted to analyze the turbulent kinetic energy [50, 51], the energy dissipation rate [51] and the power consumption [48, 51] for various mixing configurations. Other types of impellers have also been investigated. For instance, the power consumption of a pitched turbine has been analyzed [104] using a hybrid method based on the so-called blade element theory. It must be pointed out that the FVM, along with the SM technique, has also been applied in the laminar and transition regimes. We can cite, for instance, an investigation of the hydrodynamics in a coaxial mixer comprised of an anchor and a pitched blade turbine [52].

According to this literature review, it appears that the FEM and the FVM have been successfully used in a large number of mixing configurations and have been generally capable of accurately describing the hydrodynamics of a single phase in these mixing systems, particularly in local regions such as the area near the impeller. However, many industrial processes involve more than one phase, a typical example being the mixing of solid particles in a non-Newtonian polymeric

solution. The simulation process is then complicated by the coupling term between the phases and the rheological model, which generally leads to an increase in the total number of unknowns and a complexification of the system of equations to be solved. In addition, these methods often require the use of complex algorithms for parallel computations (see [46] for an example of FEM on parallel computers) and nevertheless necessitate large computational times for simulating real industrial mixing flows, resulting in a compromise between cost and accuracy. In order to reduce the complexity of the simulation procedure, it is more and more admitted that other modeling paradigms are needed.

The lattice Boltzmann method (LBM) is a powerful numerical method which has been successfully used in many research areas, such as porous media [1, 110], solid-fluid suspensions [53, 72, 111] and multiphase systems [53, 111, 112]. This method is based on the kinetic theory of gas and has been the topic of several researches in the last decade. Contrary to classical CFD approaches such as the finite element and volume methods, the Navier-Stokes equations are not directly solved with the LBM. In this case, the solution of the Navier-Stokes equations is recovered by applying a simple recurrence equation made up of two steps: the collision and the propagation steps of particles along the bonds of a lattice grid representing the computational domain. As a result, the only required computations are done during the collision step and are simple and fully local. For the propagation step, the information is directly translated from one lattice node to the neighboring lattice nodes. Thus, when this method is applied on a Cartesian structured mesh, the parallelization of the scheme is straightforward and the parallel efficiency is highly favorable.

The main difference between the LBM and classical CFD methods is the physical scale. By considering the flow at the mesoscopic scale, the primary variable of the LBM is a population of fluid particles. This change of scale presents several advantages, such as an easier way to define turbulence models [86, 113, 114], to model non-Newtonian flows [54, 115, 116] or to simulate multiphase flows [53, 111, 112], yet unfortunately it reveals a difficulty when imposing boundary conditions on macroscopic variables. In the case of homogeneous Dirichlet boundary conditions (i.e. zero velocity) on a straight wall, this limitation can be circumvented by using the so called bounce-back rule [58, 71, 72], although from a more general perspective, the imposition of non-zero velocities along arbitrarily curved surfaces is still an open topic (this point will be discussed in section 4.2.4). Nevertheless, using the adaptive force field technique [80], which belongs to the

class of the immersed boundary methods, the LBM has been successfully used to simulate the hydrodynamics of a Rushton turbine in the turbulent regime [86]. This simulation process has been used to simulate Newtonian [86, 117], Bingham [27] and thixotropic [54] fluids in order to quantify the turbulent kinetic energy [86, 117], the apparent viscosity [27] and the volume of caverns [27]. From these results, the LBM appears to be a promising method for the simulation of mixing systems. However, in the case of viscous mixing, close clearance impellers are generally used, and this smaller wall clearance leads to stronger impeller-wall interactions, which can only be captured by a geometrically flexible and numerically accurate treatment of the boundary conditions.

In order to select the most suitable boundary condition strategy, several comparisons have already been made for simple geometries. For example, the capacity to generate a zero slip velocity and to conserve the second order accuracy in space of the LBM have been studied in the case of Poiseuille and plane Couette flows [73]. The accuracy of the velocity field and the conservation of the total mass have also been investigated for an impulsively started circular flow [118]. In addition, the accuracy of the imposition of a no-slip boundary condition and the influence of the inherent parameters have been assessed for the 2D circular Couette flow [74]. From these investigations, it appears that the choice of the boundary condition strategy can highly impact the velocity at the boundary, the global accuracy of the velocity field and the order of convergence of the LBM. The objective of this work is then to assess the suitability of different strategies for imposing boundary conditions for the lattice Boltzmann method (LBM) in the case of the 3D simulation of viscous mixing flows. To our knowledge, no such comparison has been made for such complex 3D flow problems. The conclusions of this work are not limited to mixing flows and may be applicable to other types of geometrically complex flow problems.

The organization of the paper is as follows: in Section 4.2.3, the LBM is recalled and the specifications of the implementation used in this work are described. In Section 4.2.4, three commonly used strategies for imposing boundary conditions are explained. In addition, the modifications required for their implementation into a parallel LBM scheme are presented. In Section 4.2.5, the three-dimensional Couette flow is used to analyze the order of convergence of these boundary condition strategies. The impacts of the parameters inherent to these techniques are also investigated. In Section 4.2.6, a highly parallel lattice Boltzmann scheme is used to simulate the hydrodynamics of the anchor and the Paravisc (Ekato GmbH) impellers. The

accuracy of the different strategies is quantified using two macroscopic characteristic numbers, which are the power number and the pumping rate. Finally, in Section 4.2.7, the parallel performance of every boundary condition strategy is discussed and its impacts on the workload balance as well as the memory usage are analyzed.

4.2.3 The lattice Boltzmann method

The lattice Boltzmann method [58, 61, 119, 120] is based on the kinetic theory of gas and comes from the discretization in space, velocity and time of the Boltzmann equation. Only a brief presentation of the method is given here and the reader is referred to [58] for more detailed explanations. Basically, the idea is to obtain the macroscopic flow from the behaviour of a large number of microscopic particles that propagate and collide along the bonds of a lattice grid representing the computational domain. Thus, the primitive variable $f_k(\vec{x}, t)$ is mesoscopic and describes a population (or a probability density function) of particle at position $\vec{x}$, with velocity $\vec{e}_k$, at time t. The macroscopic variables can be easily recovered from the populations as the following relations define the density and the velocity:

$$\rho(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t) \tag{4.1}$$

$$\vec{u}(\vec{x}, t) = \frac{1}{\rho} \sum_{k=0}^{q-1} f_k(\vec{x}, t)\, \vec{e}_k \tag{4.2}$$

where q is the total number of populations per lattice.

With this method, the solution of the Navier-Stokes equations can be recovered by successively applying the following collision and propagation steps:

$$f_k(\vec{x}, t_+) = f_k(\vec{x}, t) + \Omega_k\big(f(\vec{x}, t)\big) \tag{4.3}$$

$$f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) = f_k(\vec{x}, t_+) \tag{4.4}$$

where Ω_k is the collision operator, as discussed below.

This means that, after collision, the populations are propagated along the direction defined by $\vec{e}_k$ during a time step δt. Here, t_+ corresponds to the time just after the collision step. The lattice grid discretization, which is Cartesian and regular, is based on the lattice spacing δx. In the present work, the D3Q15 lattice [63] is chosen and the velocities are defined as follows:

$$\vec{e}_k = \frac{\delta x}{\delta t} \begin{cases} (0,0,0) & if\ k = 0 \\ (\pm 1,0,0),(0,\pm 1,0)\ or\ (0,0,\pm 1) & if\ k = 1,6 \\ (\pm 1,\pm 1,\pm 1) & if\ k = 7,14 \end{cases} \qquad (4.5)$$

From these definitions, it can be observed that the collision step only requires local computations, and the propagation step is simply a translation of information along a structured grid. This is why the LBM can be parallelized efficiently.

4.2.3.1   The Bhatnagar-Gross-Krook collision model

The BGK model [60, 63] is the most commonly used collision model. It is based on a single relaxation towards the equilibrium population $f_k^{(eq)}(\vec{x}, t)$, using a relaxation parameter τ. The collision operator in (4.3) is defined as follows:

$$\Omega_k\big(f(\vec{x}, t)\big) = -\frac{1}{\tau}\left[f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t)\right] \qquad (4.6)$$

and the equilibrium population is given by:

$$f_k^{(eq)}(\vec{x}, t) = \omega_k \rho \left[1 + \frac{\vec{e}_k.\vec{u}}{c_s^2} + \frac{(\vec{e}_k.\vec{u})^2}{2c_s^4} - \frac{\vec{u}.\vec{u}}{2c_s^2}\right] \qquad (4.7)$$

where c_s is the speed of sound defined as:

$$c_s = \frac{1}{\sqrt{3}}\frac{\delta x}{\delta t} \qquad (4.8)$$

and ω_k are the weights of the corresponding populations. For the D3Q15 lattice, they are given by:

$$\omega_k = \begin{cases} \dfrac{2}{9} & if \ k = 0 \\[2mm] \dfrac{1}{9} & if \ k = 1,6 \\[2mm] \dfrac{1}{72} & if \ k = 7,14 \end{cases} \tag{4.9}$$

The relaxation parameter is related to the fluid viscosity μ by the following relation:

$$\tau = \frac{\mu}{\rho \delta t c_s^2} + \frac{1}{2} \tag{4.10}$$

With diffusive time scaling (i.e. $\delta t \propto \delta x^2$), this model has proven to be second-order accurate in space. The mathematical demonstration is derived from an asymptotic analysis [67] or a Chapman-Enskog expansion [121] and, under the hypotheses of small Mach and Knudsen numbers, the solution of the Navier-Stokes equations is recovered. In the case of the LBM, these dimensionless numbers are defined as follows [58]:

$$Ma = \frac{\|\vec{u}\|}{c_s} \tag{4.11}$$

$$Kn = \frac{\mu}{\rho L c_s} \tag{4.12}$$

where L is a characteristic length.

It must be pointed out that although more advanced models are available, the MRT [122] and the regularized LBM [123] schemes for instance, the BGK model was retained for the present study since it provides a sufficient level of accuracy, while offering a cost reduction factor of 10 or 20 percent [124] over these other models.

In this work, the relaxation parameter was set to one, so that Eq. (4.3) and (4.4) reduce to:

$$f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) = f_k^{(eq)}(\vec{x}, t) \tag{4.13}$$

The use of this value presents the advantage to reduce the memory cost, as the populations are equal to the equilibrium populations. In this case, the populations do not need to be stored, as the equilibrium function only requires the velocity vector and the density. This means that only four

real numbers per lattice need to be stored instead of fifteen. By reducing the amount of data required to apply the LBM scheme, the refinement possibilities are enhanced [2] so that the emphasis can be put on the lattice spacing rather than on the relaxation parameter. In fact, by fixing this parameter, the accuracy is not always optimal (an investigation of the influence of the relaxation parameter on accuracy can be found in [74]), although the computational time and the memory usage greatly decrease, hence a higher number of lattices can be used.

4.2.3.2 Parallel computation strategy

As mentioned in the introduction, in the special case of viscous mixing, the distance between the tank and the impeller is actually quite small compared to the size of the tank. As an accurate description of the flow inside this small wall clearance is crucial for the understanding of the mixing process, the discretization in this zone must be refined enough to capture the flow correctly. Thereupon, when applied to the rest of the volume, the discretization of the fluid zone leads to a substantially high number of lattices. Coupled with the fact that the LBM is based on an explicit scheme, which requires the use of small times steps, the parallelization of the computation is mandatory for performance.

The parallelization of the LBM, which relies on domain decomposition techniques, is briefly examined here and the reader is referred to [2] for more details. To minimize the memory usage, the solid lattice nodes (i.e. the lattices inside a solid part) are removed from the computational domain, leaving only the fluid lattice nodes to be distributed amongst the processors in such a way that the workload balance is optimal. This also minimizes the amount of data to be communicated before every new time step. Unfortunately, this further complicates the inter-process communications since the domain is no longer continuous, which implies that the advantages of a regular Cartesian mesh are often lost (i.e. straightforward determination of the neighbours of a given lattice). Moreover, as mentioned in the previous paragraph, by setting the relaxation parameter to one, the population does not need to be stored for the next iteration step, as the velocity and the density are sufficient to compute the equilibrium function. This means that the amount of data that must be transferred between processors is reduced. By virtue of these reductions of memory usage and efficient domain decomposition strategies, our code has been successfully utilized for the direct numerical simulation of porous media flows [1] using as many as 3.4 billion lattice nodes, spread among 256 cores (3.6 GHz Intel Xeon) for a computational

time lower than 12 hours. Such high parallel performance is possible thanks to the intrinsic locality and simplicity of the collision-propagation procedure. Consequently, one should keep in mind that boundary condition strategies can strongly affect the workload and increase the memory usage. We will come back to this in Section 4.2.7.

4.2.4 Boundary condition strategies

With the LBM, the macroscopic variables (velocity and density) are easy to obtain from the mesoscopic variable (population). However the inverse transformation is generally not possible. One major drawback of this difficulty concerns the definition of boundary conditions, as simulations generally require the imposition of velocity profiles along boundaries of the domain. From a practical point of view, this difficulty can be explained by the greater number of populations than the number of macroscopic variables per lattice, so that a Dirichlet boundary condition on velocity cannot be directly applied. As a result, the boundary conditions modify the populations of the corresponding lattices in order to tend to the required velocity.

In the case of homogeneous (i.e. zero) Dirichlet boundary conditions, the so-called half-way bounce-back rule [58, 71, 72] can be easily applied to the unknown populations. This rule is given by:

$$f_{k'}(\vec{x}, t + \delta t) = f_k(\vec{x}, t_+) \tag{4.14}$$

where k' corresponds to the direction opposite to $\vec{e}_k$ and the boundary (e.g. wall) is considered to be positioned at $\vec{x} + 0.5\vec{e}_k\delta t$ (see Fig. 4.1).

This rule simply reflects the outgoing populations obtained during the propagation step in order to define the unknown populations for the next collision step. Thanks to its simplicity, this boundary condition strategy has become the most popular approach for imposing no-slip (zero) velocities, as it allows for the handling of fluid domains with complex shapes without losing the locality of the scheme. Unfortunately, this approach is second-order accurate only in the case of straight walls perpendicular to one axis of the simulation reference frame and positioned exactly in the middle of two consecutive layers of lattices. This limitation generally implies a reduction to the first order of accuracy in space in the case of curved walls [73, 74].
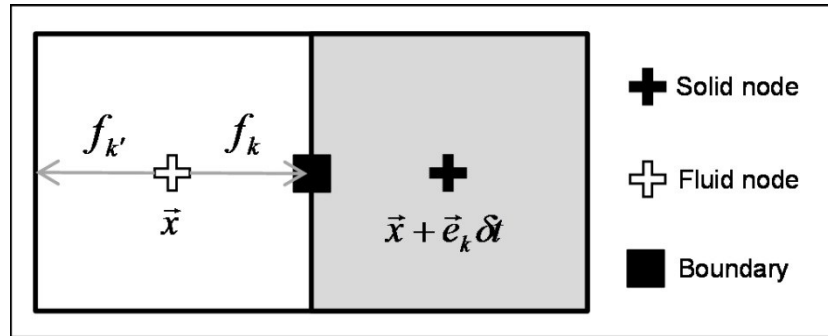
Figure 4.1: Populations used for the half-way bounce-back rule

The imposition of non-zero velocities along a complex surface is still an open topic, and several authors have proposed various boundary condition strategies based on different approaches. In order to classify them, the different methods can be split into three categories: The staircase approaches [72, 125], the interpolation or extrapolation methods [75-79, 118, 126], and the immersed boundary based methods [80-83].

In this study, three boundary condition strategies were considered: the modified bounce-back (MBB) rule proposed by Ladd [72], the extrapolation method (EM) proposed by Guo *et al.* [78] and the enforced immersed boundary-lattice Boltzmann method (IB-LBM) proposed by Wu *et al.* [83]. These methods are each representative of one category, in the sense that the MBB, independently of the shape of the boundary, uses the outgoing populations to define the unknown ones, the EM uses the distance between fluid nodes and solid parts to improve the accuracy of the boundary conditions, and the IB-LBM uses a group of control points and a corresponding body force to constrain the velocity of neighboring fluid nodes in order to mimic the motion of solid parts.

There is mention of other approaches in the literature, but they appear to be too complicated to tune and use in the case of mixing systems or other processes of similar or greater complexity (e.g. volumetric method [127, 128]) or they require a modification of the relaxation parameter (e.g. adaptive relaxation time boundary conditions [129]).

4.2.4.1 The modified bounce-back rule

The modified bounce-back (MBB) rule [72] is a classical half-way bounce-back method in which a second term, proportional to the solid part velocity $\vec{u}_b$, is used to modify the population density:

$$f_{k'}(\vec{x}, t + \delta t) = f_k(\vec{x}, t_+) - 2\omega_k \rho \frac{\vec{u}_b \cdot \vec{e}_k}{c_s^2} \tag{4.15}$$

where k' corresponds to the direction opposite to $\vec{e}_k$ and the solid part is considered to be positioned at $\vec{x} + 0.5\vec{e}_k \delta t$ (Fig. 4.2).
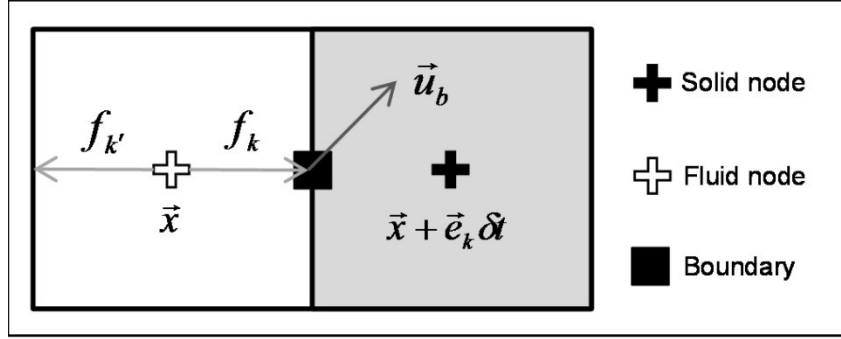
Figure 4.2: Populations used for MBB

The discretization of the solid part may be inexact, as the boundary is considered to be located midway between every couple of fluid-solid nodes. In particular, the discretization of a curved wall generates a staircase profile (see Fig. 4.3). This inaccuracy generally leads to the loss of the second order accuracy in space of the method [73, 74]. Moreover, the imposed velocity $\vec{u}_b$ itself may be treated inaccurately, as only its projection onto the direction $\vec{e}_k$ is taken into account, which means that this boundary condition strategy approximates the action of the solid part on the fluid.

However, this method is quite easy to apply for complex three-dimensional domains. First, the only requirement is to determine which lattice nodes are solid, and this task is facilitated by the intrinsic regularity of the mesh. Second, as with the regular bounce-back rule, the locality of the collision step is conserved so that there is no impact on the parallelization of the LBM itself. Finally, the utilization of this approach adds no numerical variables, as every variable in the last term of Eq. (4.15) is already known.

The localization of the solid nodes is easily achieved by determining which lattice nodes are inside the solid components of the domain. In this work, a volumetric mesh is used to discretize these solid parts into elements (or cells) and facilitate their localization. When these parts are fixed, as in the case in this work, this procedure only needs to be applied once. This preprocessing step is then negligible compared to the iterative process of the LBM.
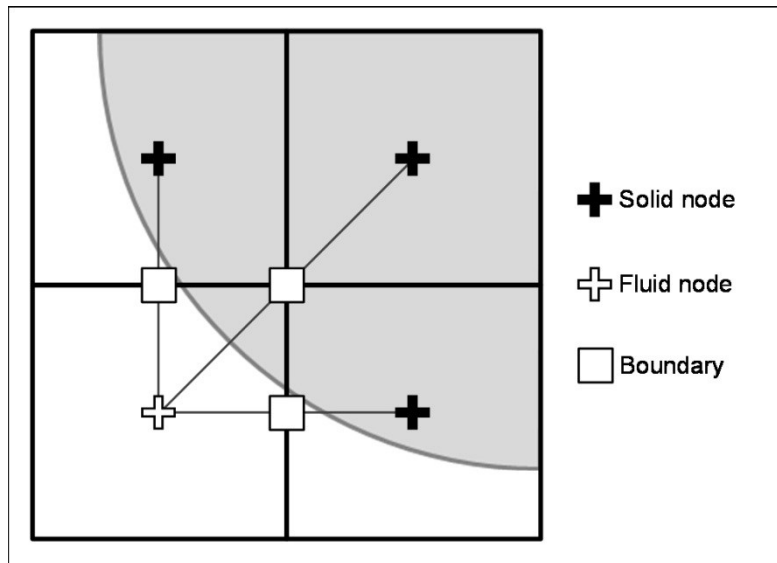
Figure 4.3: Discretization with MBB

4.2.4.2   The extrapolation method

In the extrapolation method (EM) [78], the unknown populations and their velocities are computed at solid nodes, the black crosses in Fig. 4.4, by an extrapolation procedure, using the velocity and the populations of neighboring fluid nodes and the fraction of the intersected link Δ from the solid part.
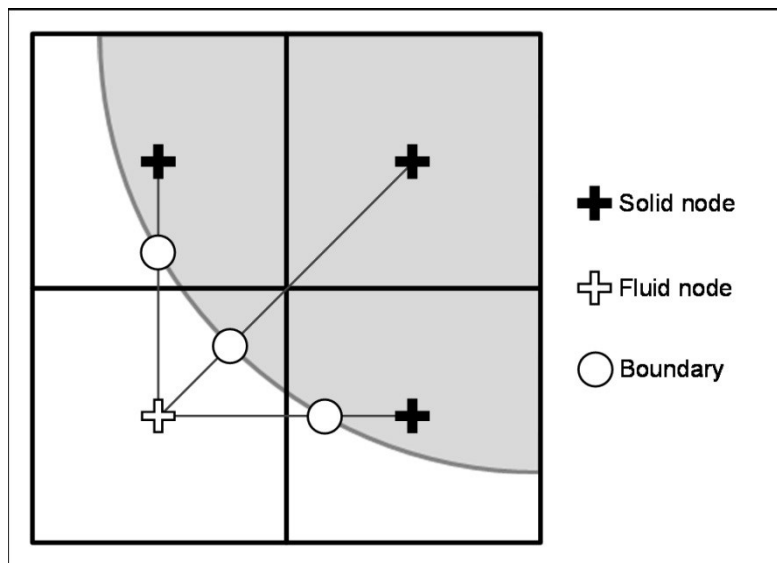
Figure 4.4: Discretization with EM

This approach allows for a more accurate shape of the solid part (see Fig. 4.4), as the boundary is no longer considered to be located midway between fluid and solid nodes (see Fig. 4.5). The fraction Δ is computed as follows:

$$\Delta = \frac{|\vec{x}_f - \vec{x}_b|}{|\vec{x}_f - \vec{x}_w|} \tag{4.16}$$

where $\vec{x}_w$, $\vec{x}_f$ and $\vec{x}_b$ correspond respectively to the position of the solid node, the fluid node and the intersection between the actual boundary and the line joining $\vec{x}_w$ and $\vec{x}_f$ (see Fig. 4.5).
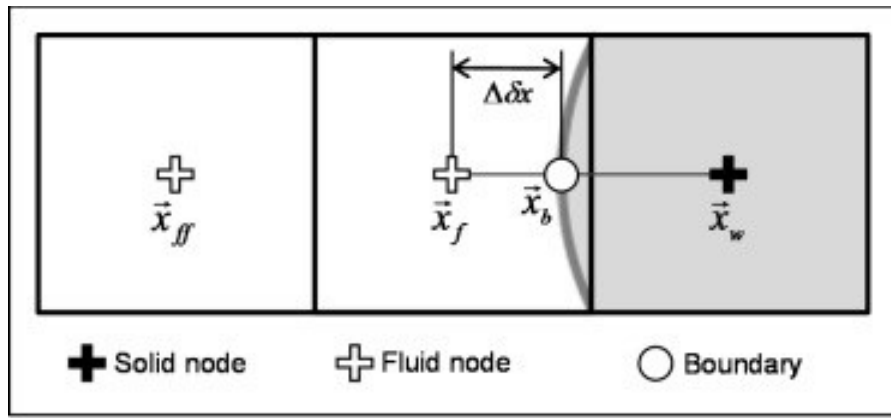
Figure 4.5: Fraction to the boundary with EM

Let us first introduce the decomposition of a population into equilibrium and non-equilibrium parts:

$$f_k(\vec{x}, t) = f_k^{(eq)}(\vec{x}, t) + f_k^{(neq)}(\vec{x}, t) \tag{4.17}$$

Using Eqs. (4.3) and (4.6), the population at solid node $\vec{x}_w$ required for the next propagation step is then given by:

$$f_k(\vec{x}_w, t_+) = \tilde{f}_k^{(eq)}(\vec{x}_w, t) + \left(1 - \frac{1}{\tau}\right) f_k^{(neq)}(\vec{x}_w, t) \tag{4.18}$$

As node $\vec{x}_w$ is solid, the two terms on the right-hand side are unphysical and must be obtained by extrapolation. First, for the equilibrium part of Eq. (4.18), the regular equilibrium function is used (see Eq. (4.7)):

$$\tilde{f}_k^{(eq)}(\vec{x}_w, t) = \omega_k \rho_w \left[1 + \frac{\vec{e}_k \cdot \vec{u}_w}{c_s^2} + \frac{(\vec{e}_k \cdot \vec{u}_w)^2}{2c_s^4} - \frac{\vec{u}_w \cdot \vec{u}_w}{2c_s^2} \right] \tag{4.19}$$

where the macroscopic variables are determined using the neighboring nodes. More precisely, the density ρ_w is approximated by $\rho(\vec{x}_f, t)$ and the velocity $\vec{u}_w$ is determined by an extrapolation procedure. Following the formulation of the extrapolation parameters proposed by Suh *et al.* [74], the velocity $\vec{u}_w$ is computed as follows:

$$\vec{u}_w = \gamma_0 \vec{u}_b + \gamma_1 \vec{u}_f + \gamma_2 \vec{u}_{ff} \tag{4.20}$$

where $\vec{u}_b$, $\vec{u}_f$ and $\vec{u}_{ff}$ correspond to the velocity at nodes $\vec{x}_b$, $\vec{x}_f$ and $\vec{x}_{ff}$, respectively, and where the extrapolation parameters γ_i are given by:

$$\gamma_0 = \begin{cases} \dfrac{3 - \Delta}{1 + \Delta} & if\ \Delta < 0.75 \\ \dfrac{1}{\Delta} & if\ \Delta \geq 0.75 \end{cases} \tag{4.21}$$

$$\gamma_1 = \begin{cases} \Delta - 1 & if\ \Delta < 0.75 \\ \dfrac{\Delta - 1}{\Delta} & if\ \Delta \geq 0.75 \end{cases} \tag{4.22}$$

$$\gamma_2 = \begin{cases} -\dfrac{(1 - \Delta)^2}{(1 + \Delta)} & if\ \Delta < 0.75 \\ 0 & if\ \Delta \geq 0.75 \end{cases} \tag{4.23}$$

Second, the non-equilibrium part of Eq. (4.18) is directly extrapolated from the neighboring nodes:

$$f_k^{(neq)}(\vec{x}_w, t) = \beta f_k^{(neq)}(\vec{x}_f, t) + (1 - \beta) f_k^{(neq)}(\vec{x}_{ff}, t) \tag{4.24}$$

where the extrapolation parameter β is given by:

$$\beta = \begin{cases} \Delta & if\ \Delta < 0.75 \\ 1 & if\ \Delta \geq 0.75 \end{cases} \tag{4.25}$$

Based on these definitions, it can be observed that this boundary condition strategy relies on four different extrapolation parameters: γ_0, γ_1, γ_2 and β. These parameters are local (i.e. different for every lattice and every direction) and only depend on the fraction Δ (see Eq. (4.21), (4.22), (4.23) and (4.25)). Henceforth in this paper, this formulation will be referred as the original EM formulation.

As proposed by Suh *et al.* [74], the extrapolation parameters γ_0, γ_1, γ_2 and β can be considered as free numerical parameters. They showed that, for a given geometry, one can optimize them in order to minimize the error and/or improve the stability. By means of an analysis of the slip velocity on a straight wall, they found the following relations:

$$\gamma_0 = 1 - \gamma_1 - \gamma_2 \tag{4.26}$$

$$\gamma_2 = \frac{\Delta}{1 + \Delta}(2 - \gamma_1) - 1 \tag{4.27}$$

or, using Eq. (4.26):

$$\gamma_0 = \frac{2 - \gamma_1}{1 + \Delta} \tag{4.28}$$

As a result, in such a case, only γ_1 and β can considered free. In that they are also global (i.e. constant for all lattices and directions), one can choose values of these parameters that will maximize the accuracy and/or the stability of the LBM scheme.

As previously mentioned, the relaxation parameter τ is fixed to one in this work. This implies that the last term of Eq. (4.18) vanishes, and only the equilibrium part of the populations is needed. Consequently, the extrapolation parameter β of the non-equilibrium part is no longer useful, which means that the only free parameter is γ_1. Throughout the rest of this work, this formulation will be referred to as the free EM formulation.

It is worth noting that, for both the original and free EM formulations, extrapolation parts of the boundary condition strategy, that is the computation of $\vec{u}_w$ using Eq. (4.20) and the computation of $f_k^{(neq)}(\vec{x}_w, t)$ using Eq. (4.24), imply that the boundary condition strategy is no longer local. Nevertheless, by computing $\vec{u}_w$ and $f_k^{(neq)}$ when treating the collision-propagation step of the first fluid node $\vec{x}_f$, no modification is required in the data structure of the LBM code.

Additionally, it eliminates the need to increase the amount of data communicated between related processors, as the information transmitted for the next collision-propagation iteration is sufficient to compute the boundary conditions.

In the same way as the MBB rule, the solid nodes need to be identified, therefore volumetric meshes are also used to determine them by selecting all the lattice nodes situated inside one element of the mesh. This boundary condition strategy also requires determining the fraction Δ for every couple of solid-fluid lattice nodes. Even if these fractions are not additional numerical parameters, in the sense they are only related to geometrical aspects, their computation can be rather time consuming. For simple solid parts, such as planes or cylinders, the computation can be done analytically as the intersection between the line defined by $\vec{e}_k$ and the equation of such a part leads to solving a linear or quadratic polynomial equation. In the case of geometrically complex objects, such as impellers, analytical parameterizations of the boundary shape are rarely available. In this work, the impeller surfaces are defined by surface meshes of boundary elements, implying the use of a search algorithm to find the elements intersecting the related directions defined by the couples of solid-fluid lattice nodes. In each case, the coordinates $\vec{x}_b$ of the boundary, which are used in the fraction computation (Eq. (4.16)), are the intersection of the line defined by $\vec{e}_k$ and the corresponding surface element of the mesh. Once again, in the case of a Lagrangian frame of reference, the computation of the fraction only has to be done once since the solid parts are fixed. The impact of the fraction computations on the computational time will be addressed in Section 4.2.7.

Finally, we have observed that, for some specific configurations, the boundary condition can be ill-defined with this technique. This occurs when two opposite directions for the same lattice point towards solid walls. In this case, the extrapolated velocities (Eq. (4.20)) at the later solid nodes cannot be computed as the velocity of the second fluid node, located at $\vec{x}_{ff}$, is not defined. When this happens, the velocity of the solid part is directly used instead, without extrapolation.

4.2.4.3 The immersed boundary – lattice Boltzmann method

With classical CFD methods, immersed boundary methods consider a fully fluid domain in which the fluid velocity is constrained at various control points representing the immersed solid part. The boundary condition is then enforced by modifying the velocity of neighboring nodes in order to tend to the required velocity. When using the LBM, the velocity is not a primitive variable; the

immersed boundary-lattice Boltzmann method (IB-LBM) [83] enforces a velocity $\vec{u}_b$ on control points by means of a body force (see Fig. 4.6).
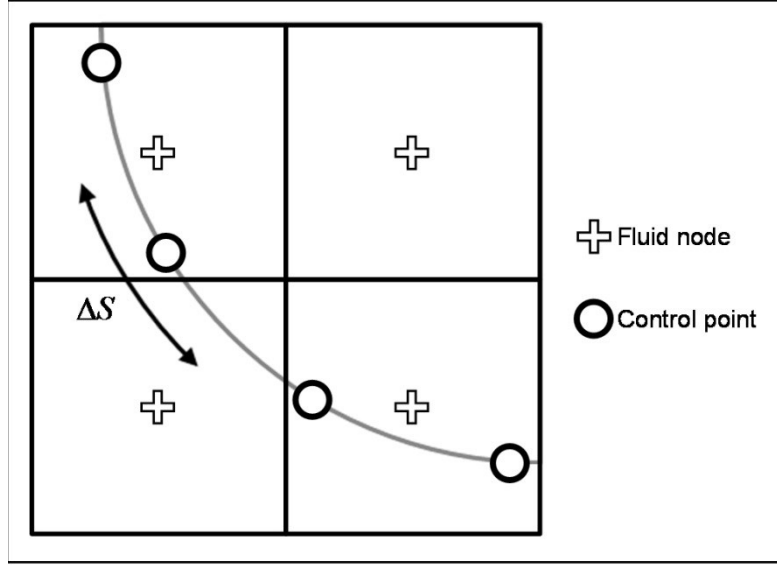
Figure 4.6: Example of control point distribution with IB-LBM

Let us first introduce the body force formulation proposed by Guo *et al.* [65], which can be written as:

$$f_k(\vec{x}, t_+) = \left(1 - \frac{1}{\tau}\right) f_k(\vec{x}, t) + \frac{1}{\tau} f_k^{(eq)}(\vec{x}, t) + F_k(\vec{x}, t)\delta t \tag{4.29}$$

with

$$F_k(\vec{x}, t) = \left(1 - \frac{1}{2\tau}\right) \omega_k \left(\frac{\vec{e}_k - \vec{u}}{c_s^2} + \frac{\vec{e}_k.\vec{u}}{c_s^4}.\vec{e}_k\right).\vec{g}(\vec{x}, t) \tag{4.30}$$

$$\rho\vec{u}(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t)\,\vec{e}_k + \frac{\delta t}{2}\,\vec{g}(\vec{x}, t) \tag{4.31}$$

where the body force $\vec{g}$ is now derived.

Following Eq. (4.31), the velocity can be decomposed as:

$$\vec{u} = \vec{u}^* + \delta\vec{u} \tag{4.32}$$

where the intermediate velocity $\vec{u}^*$ is given by:

$$\rho\vec{u}^* = \sum_{k=0}^{q-1} f_k\,(\vec{x},t)\vec{e}_k \tag{4.33}$$

so that the body force $\vec{g}$ can be expressed as a function of the velocity correction $\delta\vec{u}$:

$$\vec{g} = \frac{2\rho\delta\vec{u}}{\delta t} \tag{4.34}$$

The body force is then proportional to the velocity correction $\delta\vec{u}$, which is a priori unknown but can be related to the velocity correction $\delta\vec{u}_c$ at the neighboring control points.

Let us now consider a group of m control points and their respective coordinates $\vec{X}_c(s_i,t) = (X_c(s_i,t), Y_c(s_i,t), Z_c(s_i,t)), i = 1,2,\dots,m$ where s_i is the Lagrangian parametric coordinate. We associate with every control point i an unknown velocity correction $\delta\vec{u}_c(\vec{X}_c(s_i,t),t)$.

In order to couple the velocity corrections $\delta\vec{u}$ and $\delta\vec{u}_c$, the Dirac function $\delta(r)$ is introduced, which is approximated by [9, 85]:

$$\delta(r) = \begin{cases} \dfrac{1}{4}\left(1 + \cos\left(\dfrac{\pi r}{2}\right)\right) & if\,|r| \le 2 \\ 0 & otherwise \end{cases} \tag{4.35}$$

This function can be extended to vector $\vec{x} - \vec{X}_c(s_i,t)$:

$$D\left(\vec{x} - \vec{X}_c(s_i,t)\right) = \frac{1}{\delta x^3}\,\delta\left(\frac{x - X_c(s_i,t)}{\delta x}\right)\delta\left(\frac{y - Y_c(s_i,t)}{\delta x}\right)\delta\left(\frac{z - Z_c(s_i,t)}{\delta x}\right) \tag{4.36}$$

The velocity correction $\delta\vec{u}$ at a lattice node can then be approximated as:

$$\delta\vec{u}(\vec{x},t) = \sum_{i=1}^{m} \delta\vec{u}_c(\vec{X}_c(s_i,t),t)D\left(\vec{x} - \vec{X}_c(s_i,t)\right)\Delta S_i \tag{4.37}$$

where ΔS_i is the arc length (in 2D) or the area (in 3D) of the boundary element inside of which the control point i is located (see Fig. 4.6 for an example in 2D).

The next step consists of relating $\delta \vec{u}_c$ to the velocity at the control points $\vec{u}_c$, the velocity at the fluid nodes $\vec{u}$, and the velocity of the solid part $\vec{u}_b$. To do so, $\vec{u}_c$ at the control point i is interpolated using the Dirac function of Eq. (4.36):

$$\vec{u}_c\big(\vec{X}_c(s_i,t),t\big) = \sum_{\vec{x}\in\Omega} \vec{u}(\vec{x},t) D\left(\vec{x} - \vec{X}_c(s_i,t)\right)\delta x^3 \tag{4.38}$$

where Ω is the computational domain.

By substituting Eq. (4.32) into Eq. (4.38), the following relation is obtained:

$$\vec{u}_c\big(\vec{X}_c(s_i,t),t\big) = \sum_{\vec{x}\in\Omega} \vec{u}^*(\vec{x},t) D\left(\vec{x} - \vec{X}_c(s_i,t)\right)\delta x^3$$
$$+ \sum_{\vec{x}\in\Omega} \delta\vec{u}(\vec{x},t) D\left(\vec{x} - \vec{X}_c(s_i,t)\right)\delta x^3 \tag{4.39}$$

or, using Eq. (4.37):

$$\vec{u}_c\big(\vec{X}_c(s_i,t),t\big) = \sum_{\vec{x}\in\Omega} \vec{u}^*(\vec{x},t) D\left(\vec{x} - \vec{X}_c(s_i,t)\right)\delta x^3$$
$$+ \sum_{\vec{x}\in\Omega}\sum_{j=1}^{m} \delta\vec{u}_c\big(\vec{X}_c(s_j,t),t\big) D\left(\vec{x} - \vec{X}_c(s_j,t)\right)\Delta S_j\, D\left(\vec{x} - \vec{X}_c(s_i,t)\right) \tag{4.40}$$

As the goal of the method is to enforce the velocity of the solid part on the control points, $\vec{u}_c$ is then replaced by $\vec{u}_b$:

$$\vec{u}_b\big(\vec{X}_c(s_i,t),t\big) - \sum_{\vec{x}\in\Omega} \vec{u}^*(\vec{x},t) D\left(\vec{x} - \vec{X}_c(s_i,t)\right)\delta x^3$$
$$= \sum_{\vec{x}\in\Omega}\sum_{j=1}^{m} \delta\vec{u}_c\big(\vec{X}_c(s_j,t),t\big) D\left(\vec{x} - \vec{X}_c(s_j,t)\right)\Delta S_j\, D\left(\vec{x} - \vec{X}_c(s_i,t)\right)\delta x^3 \tag{4.41}$$

Considering that Eq. (4.41) is valid for every control point, two vectors are next introduced, the unknown correction vector $\vec{\varphi}$ and the objective vector $\vec{b}$:

$$\vec{\varphi}_i = \delta\vec{u}_c\big(\vec{X}_c(s_i,t),t\big), \forall\, i \in [1,m] \tag{4.42}$$

$$\vec{b}_i = \vec{u}_b\big(\vec{X}_c(s_i,t),t\big) - \sum_{\vec{x}\in\Omega}\vec{u}^*(\vec{x},t)D\big(\vec{x} - \vec{X}_c(s_i,t)\big)\delta x^3, \forall\, i \in [1,m] \tag{4.43}$$

The substitution of Eq. (4.42) and (4.43) into Eq. (4.41) leads to the following system of linear equations:

$$A\vec{\varphi} = \vec{b} \tag{4.44}$$

where

$$A_{ij} = \sum_{\vec{x}\in\Omega}D\big(\vec{x} - \vec{X}_c(s_j,t)\big)\Delta S_j D\big(\vec{x} - \vec{X}_c(s_i,t)\big)\delta x^3, \forall\, i,j \in [1,m] \tag{4.45}$$

By definition the matrix A solely depends on the lattice spacing δx and the coordinates of the control points, which implies that this matrix only have to be computed once for a fixed solid part. In addition, when applied to a large number of control points, the size of the system becomes crucial. The conjugate gradient method is used in this work since it outperforms direct methods both in terms of memory and CPU time when the size of the system becomes large, which is often the case for industrial problems. Note that this part of the computation has not been parallelized.

At this point, the boundary condition is entirely defined. Indeed, solving the system of equations (44) yields the velocity correction $\delta\vec{u}_c$ at the control points. The velocity correction $\delta\vec{u}$ at the lattice nodes is then computed through Eq. (4.37) and used to correct the velocity in Eq. (4.32). Finally, the body force $\vec{g}$, which can be computed easily from to the velocity correction $\delta\vec{u}$ with Eq. (4.34), is applied in the collision step of Eq. (4.29). This procedure is summarized in the following algorithm [83]:

1) Compute matrix A with Eq. (4.45) (only at $t = 0$ in case of fixed objects);
2) Apply the collision-propagation scheme involving the body force $\vec{g}$, as defined in Eq. (4.29) ($\vec{g}(\vec{x}, 0) = 0$), and compute macroscopic variables ρ and $\vec{u}^*$ with Eq. (4.1) and Eq. (4.33);
3) Compute vector $\vec{b}$ defined by Eq. (4.43);
4) Solve the linear system of Eq. (4.44) to obtain the correction $\delta\vec{u}_c$ at the control points and use Eq. (4.37) to compute the correction $\delta\vec{u}$ at the fluid nodes and Eq. (4.34) to compute the body force $\vec{g}$;
5) Correct the velocity at the lattices with Eq. (4.32) and compute the external force using Eq. (4.30);
6) Compute the equilibrium function defined by Eq. (4.7);
7) Move the control points (in case of moving objects);
8) Repeat step 1 to step 7 until convergence is reached.

Owing to this approach, a velocity profile can be imposed at the surface of a solid part with the use of a surface mesh. Unfortunately, because this method is intrinsically global, the locality of the LBM scheme is not preserved. First, this method requires solving a system of equations, which increases the computational time, and implies additional communications between processors. The impact on the parallel efficiency and the memory usage will be addressed in Section 4.2.8. Second, during the interpolation and spreading steps (Eqs. (4.38) and (4.37)), the exchange of information between lattice nodes and control points is obviously not local. In order to reduce the impact of these two steps, another approximation of the Dirac function is used in this work [130]:

$$\delta(r) = \begin{cases} \frac{1}{6}\left(5 - 3|r| - \sqrt{-3(1 - |r|)^2 + 1}\right) & 0.5 \leq |r| \leq 1.5 \\ \frac{1}{3}\left(1 + \sqrt{-3r^2 + 1}\right) & |r| \leq 0.5 \\ 0 & otherwise \end{cases} \tag{4.46}$$

which reduces the support of the function from 4 to 3. The major advantage of this reduction is that, for a given control point, the neighboring lattice nodes are the same as those required for the propagation step, thus no modification in the data structure of the LBM program is required.

Finally, in order to prevent dimensional problem with the term ΔS_i of Eq. (4.37), we propose the following definition:

$$\Delta S_i = \Delta S \delta x^3 \tag{4.47}$$

with

$$\Delta S = \frac{S_{part}}{m \delta x^2} \tag{4.48}$$

where S_{part} denotes the surface of the solid part and m is the total number of control points.

In this definition, the term ΔS has the advantage to be related to the total number of control points and the lattice spacing. This point will be highlighted in Section 4.2.5.2

4.2.5 Convergence study

In order to verify the order of convergence of the boundary condition strategies proposed in the previous section, the three-dimensional Couette flow is analyzed. Given that this flow can be seen as a simplified mixer (i.e. with a centered cylindrical impeller), the conclusions are of interest with regard to mixing simulations. Moreover, its simplicity permits the analysis of the boundary condition parameters and helps to select them properly for real industrial mixing systems.

4.2.5.1 Convergence study

This problem has the advantage of possessing an analytical solution even if the boundaries are curved. In this work, the inner cylinder is rotating and the outer is fixed (Fig. 4.7).
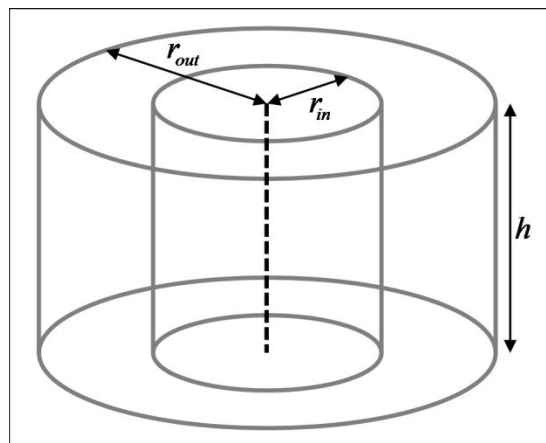
Figure 4.7: Couette flow geometry

In the case of a Newtonian liquid, the analytical solution in the laminar regime is expressed as:

$$\vec{u}^* = u_\theta^*(r)\vec{e}_\theta \qquad (4.49)$$

with

$$u_\theta^*(r) = \omega \frac{(r_{in}r_{out})^2}{(r_{out}^2 - r_{in}^2)} \left(\frac{1}{r} - \frac{r}{r_{out}^2}\right) \qquad (4.50)$$

where r_{in}, r_{out} and ω correspond to the inner radius, the outer radius and the angular velocity.

The error e between the analytical solution and the simulated velocity field can be evaluated as:

$$e = \sqrt{\frac{1}{n_{tot}} \sum_{i=1}^{n_{tot}} \left(\frac{|\vec{u}_i - \vec{u}_i^*|^2}{u_{char}^2}\right)} \qquad (4.51)$$

where n_{tot} corresponds to the total number of fluid lattice nodes and $u_{char} = \omega r_{in}$ is a characteristic tangential velocity. Concerning the simulation with the IB-LBM, only the lattice nodes between the inner and the outer radii are taken into account for the error computation, even though every lattice node in the domain is considered a fluid node with this method.

The Reynolds number associated with the Couette flow problem, in the case of a Newtonian fluid, is defined as:

$$Re = \frac{\rho \omega r_{in}(r_{out} - r_{in})}{\mu} \qquad (4.52)$$

4.2.5.1.1 Configuration

We consider a Couette geometry defined by the following parameters: $r_{in} = 0.1\ m$, $r_{out} = 0.2\ m$ and $h = 8\delta x$. As the flow is independent of the axial coordinates, the number of lattices in this direction ($\vec{z}$) is fixed to eight in order to reduce the computational time for the finest meshes. The total number of processors is fixed to two, the domain is split up into two subdomains along the z axis and there are thus four layers of lattices per processor.

To determine the impact of the three boundary condition strategies on the order of convergence of the LBM, four different lattice spacings were used. Their values are:

$$\delta x \in [1; \ 0.5; \ 0.25; \ 0.125] * 10^{-2} m \tag{4.53}$$

The impact of the Reynolds number on the error is also investigated. The selected Reynolds numbers belong to the laminar regime and their values are:

$$Re \in [10^{-3}; \ 10^{-1}; \ 10] \tag{4.54}$$

The corresponding angular velocities can be obtained by Eq. (4.52).

As specified in Section 4.2.3, the relaxation parameter τ is set to one, so the time step δt is directly computed from the lattice spacing and the viscosity. Using Eq. (4.8), Eq. (4.10) becomes:

$$\delta t = \frac{\rho \delta x^2}{6\mu} \tag{4.55}$$

The numerical parameters associated with every boundary condition strategy were defined in Section 4.2.4. For the EM, the fractions are computed using the exact equation of the cylinders and the extrapolation parameters only depend on these fractions, as proposed by Guo *et al.* [78]. For the IB-LBM, a uniform control point distribution is used and its determination is highlighted in Section 4.2.5.2. The boundary conditions for the top and bottom of the domain are periodic.

Finally, in order to accurately compare the errors obtained from different lattice spacings and Reynolds numbers, a general stopping condition is needed. After conducting different tests, it appears that the following condition is appropriate since it adapts to the flow conditions and lattice spacing:

$$\frac{\Delta u}{u_{char}} \frac{l_{char}}{\delta x} < \varepsilon \tag{4.56}$$

where ε is a given tolerance and l_{char} is the characteristic length.

For the Couette flow problem, $u_{char} = \omega r_{in}$ and $l_{char} = r_{in}$, therefore the condition reduces to:

$$\frac{\Delta u}{\omega \delta x} < \varepsilon \qquad (4.57)$$

The velocity variation Δu is the difference between two consecutive average velocities, which is required to eliminate oscillations [72]:

$$\Delta u = \tilde{u}(t) - \tilde{u}(t - \delta t) \qquad (4.58)$$

with

$$\tilde{u}(t) = \frac{u_{avg}(t) + u_{avg}(t - \delta t)}{2} \qquad (4.59)$$

where

$$u_{avg}(t) = \frac{1}{n_{tot}} \sum_{i=1}^{n_{tot}} |\vec{u}_i(t)| \qquad (4.60)$$

For the Couette flow problem, the average velocity u_{avg} is computed using the cylindrical components of the velocity (i.e. $u_r = u_x \frac{x}{r} + u_y \frac{y}{r}$, $u_\theta = u_y \frac{x}{r} - u_x \frac{y}{r}$ and u_z).

In this work, the tolerance ε was fixed at 10^{-10} for accuracy reasons. It is obvious that such a low value of ε significantly increases the computational time but, in this section, the emphasis is put on the accuracy rather than on the computational time.

4.2.5.1.2 Results

The evolution of the error versus the lattice spacing for the three Reynolds numbers is presented in Fig. 4.8(a) for the modified bounce-back rule (MBB), in Fig. 4.8(b) for the extrapolation method (EM) and in Fig. 4.8(c) for the immersed boundary-lattice Boltzmann method (IB-LBM). From Fig. 4.8(a), it appears that the MBB affects the order of convergence of the LBM by reducing it to slightly above one. This reduction has already been observed [73, 74] and can be explained by the inexact discretization of the cylinders. Equally interesting is that the results are not affected by the Reynolds number in the range of values considered. The results of Fig. 4.8(b) show that the extrapolation method is capable of conserving the second order accuracy of the LBM, and the accuracy is hardly affected by the Reynolds number. Finally, from Fig. 4.8(c), it

seems that the use of the IB-LBM, as in the case of the MBB, leads to a reduction in the order of convergence. It is important to mention that a previous study showed that the IB-LBM is second order accurate when applied to the decaying vortex problem [83]. This difference can be explained by the fact that the flow is not driven by the boundary conditions, as the IB-LBM was only used to perturb the flow. Moreover, note that the IB-LBM also affects the stability of the LBM scheme. One way to assess this stability consists of determining the maximum Mach number (or equivalently the maximum Reynolds number, since the relaxation number is fixed to 1 in this work) that can be simulated in a stable manner with the IB-LBM as well as the other two boundary condition strategies. Our tests have revealed that the maximum Mach numbers with the MBB and the EM are close to 0.3. Conversely, this maximum value was reduced to 0.1 with the IB-LBM. As a result, all simulations were divergent for $Re = 10$ with the IB-LBM.
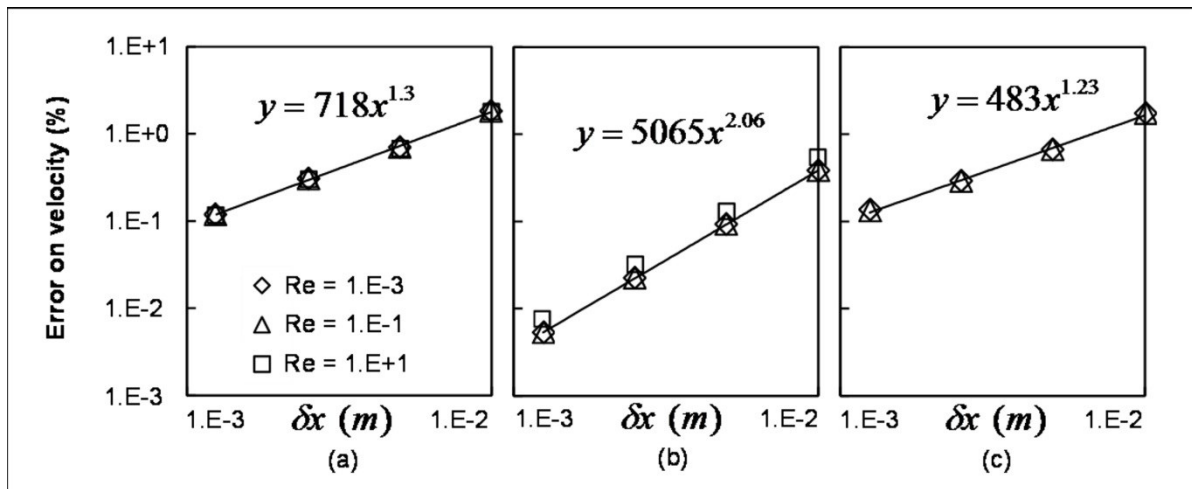
Figure 4.8: Convergence study for the Couette flow problem with (a) the MBB, (b) the EM and (c) the IB-LBM

In conclusion, it appears from Fig. 4.8 that the EM is the most accurate approach and is the only strategy capable of conserving the second order accuracy of the LBM scheme for this Couette flow problem. The results obtained with the MBB and the IB-LBM are similar although less accurate than those obtained with the EM. Furthermore, convergence profiles indicating first-order accuracy are observed with these two techniques.
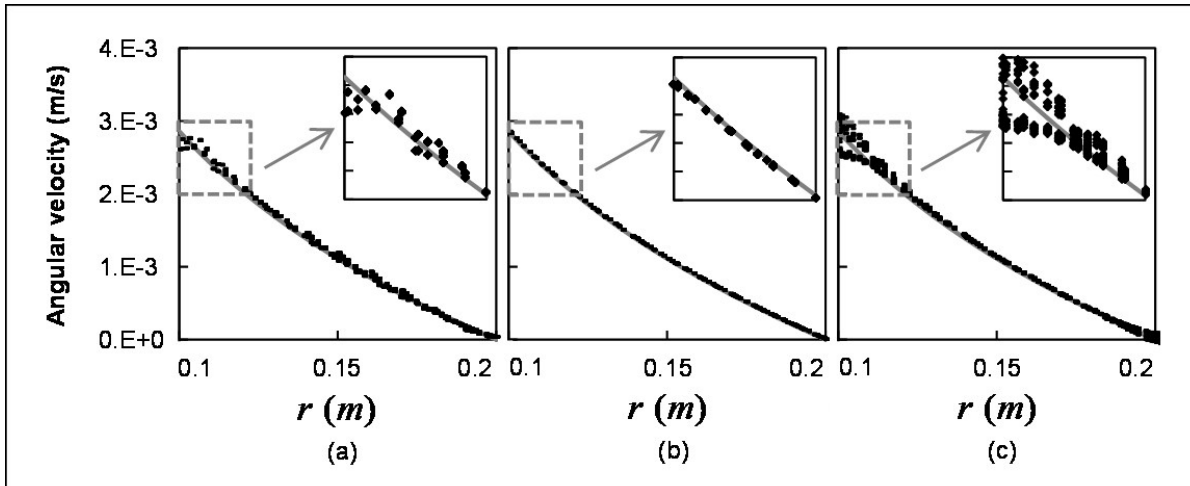
Figure 4.9: Angular velocity profiles obtained with (a) the MBB, (b) the EM and the (c) IB-LBM. The grey line represents the analytical solution

In order to better understand the differences in accuracy, the angular velocity profiles and the corresponding local errors are analyzed. In Fig. 4.9, the velocity profiles with the lattice spacing $\delta x = 10^{-2} \, m$ are plotted for the three boundary condition strategies. From Fig. 4.9(a), it appears that the simulated profile with the MBB oscillates around the analytical solution. In addition, these oscillations are observed in the entire domain, even if they appear to be slightly higher near the inner radius. For the EM (Fig. 4.9(b)), the simulated profile fits accurately with the analytical solution. For the IB-LBM (Fig. 4.9(c)), the simulated profile globally coincides with the analytical solution, except near the boundaries at $r = 0.1$ and 0.2 where oscillations can be observed.

In Fig. 4.10, the average local errors on the angular velocity (i.e. the average error with respect to the radius) with the lattice spacing $\delta x = 10^{-2} \, m$ are plotted for the three boundary condition strategies. According to Fig. 4.10(a), it appears that the error profile with the MBB is quite sensitive to the radius, which comes from the fact that the solution is perturbed by oscillations, as observed in Fig. 4.9(a). For the EM in Fig. 4.10(b), the error remains very small and rather constant despite a slight increase near the inner radius. Finally, with the IB-LBM, it can be observed in Fig. 4.10(c) that the global error is clearly dominated by errors near the inner radius. These results signify that, with the three boundary conditions approaches, the maximum error is situated near the boundary where a non-zero velocity is imposed.
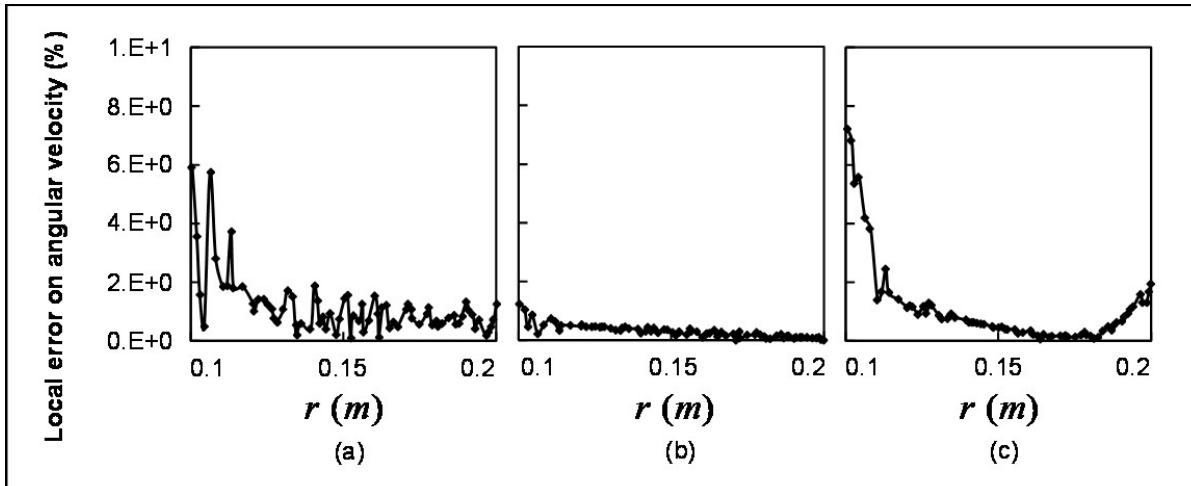
Figure 4.10: Average local error profiles with (a) the MBB, (b) the EM and (c) the IB-LBM

4.2.5.2 Boundary conditions parameters

As discussed in Section 4.2.4, only the EM and the IB-LBM require numerical parameters. For the EM, the extrapolation parameters can be seen as free parameters that are chosen to minimize the error. Since the surface of a solid part cannot be generally described by an analytical expression, the impact of its discretization needs to be investigated. In the same manner, the effect of the control point distribution for the IB-LBM needs to be analyzed.
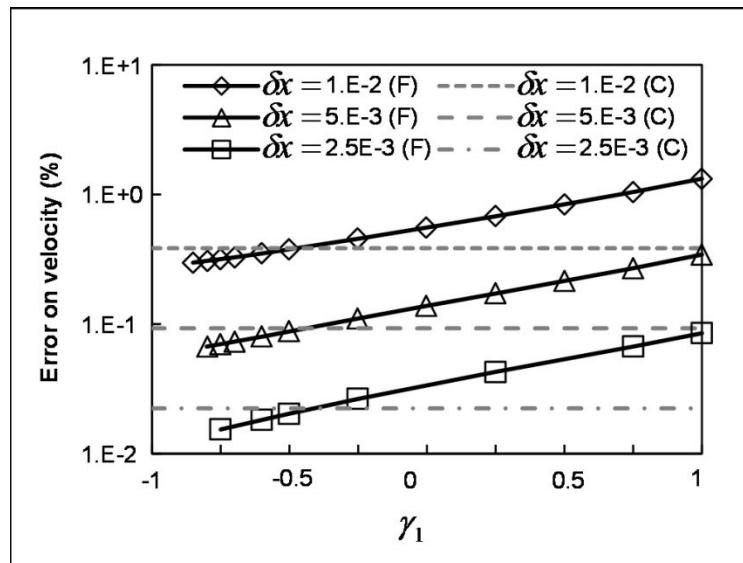
Figure 4.11: Error study on the extrapolation parameter of the EM [(F) refers to the use of the free parameter; (C) refers to the regular definition]

As seen in Section 4.2.4.2, the use of the free formulation [74] for the extrapolation parameters in the EM, for the special case $\tau = 1$, reduces the total number of numerical parameters to one. Thus, only the free parameter γ_1 needs to be selected. Fig. 4.11 compares the variation of the error on velocity with respect to γ_1 (F) to the results obtained by the regular definition (C) proposed by Guo *et al.* [78]. Given that the impact of the Reynolds number is negligible, the study is limited to $Re = 10^{-1}$. From these profiles it appears that, regardless of the lattice spacing, only a restricted range of γ_1, the values lower than -0.5, leads to an error inferior to that with the regular definition. Unfortunately, this improvement in accuracy is combined with a reduction in stability, which is amplified for fine lattice spacings. In order to conserve the stability, the regular definition of the extrapolation parameters seems to be safer for the simulation of industrial mixing systems. Nevertheless, this conclusion is limited to the case $\tau = 1$, and it was shown in [74] that is possible to choose free parameters that improve significantly the accuracy of simulation results, without affecting the stability.
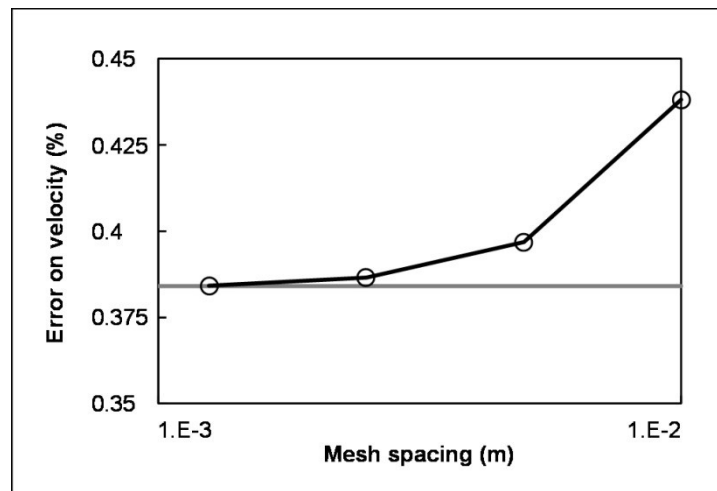
Figure 4.12: Variation of the error versus the mesh spacing for the EM (the grey line refers to the analytical fraction, the circles refer to fraction computed using a mesh)

In addition, the EM requires the computation of the fractions Δ that allow to accurately describe the shape of the solid parts. As mentioned in Section 4.2.4.2, impeller surfaces cannot be described by an analytical equation, so that meshes are used in order to do so. This means that such a discretization is included in the boundary condition strategies, and its impact therefore needs to be analyzed. The Couette flow problem can be seen as the worst-case scenario, because all the boundaries are curved, meaning every fraction Δ will be affected by the discretization of

the solid parts. The variation of the error with respect to the mesh spacing is plotted in Fig. 4.12. The lattice spacing is $\delta x = 10^{-2}\, m$ and the Reynolds number is $Re = 10^{-1}$. From these profiles, it appears that the results converge to the one obtained with the analytical fraction. This result signifies that the second order accuracy of the LBM can be conserved by using fine enough obstacle mesh spacing for the solid parts.
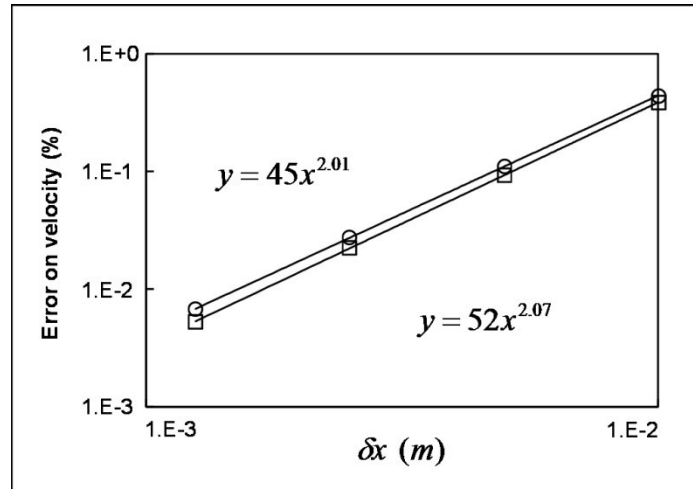
Figure 4.13: Impact of the discretization of the inner and outer cylinders on the accuracy for the EM (the squares refer to the analytical fraction, the circles refer to fraction computed using a mesh)

In practice, in order to limit the total number of nodes of the surface mesh and memory usage, it would be more convenient to link the mesh spacing to the lattice spacing. By keeping the ratio of these two spacings constant, the second order accuracy can be conserved. For example, Fig. 4.13 shows that, for a ratio equal to one, the impact of such a strategy on the accuracy is small and the second order accuracy is preserved.

In the case of the IB-LBM (Section 4.2.4.3), the obstacle is discretized in order to obtain the control point distribution, and these points are then used to enforce the velocity on the solid part. This approach requires solving a system of equations defined by Eq. (4.44), where the matrix (Eq. (4.45)) depends on the Dirac function, the coordinates of the control points and the lattice spacing. Given that the Dirac function has been chosen (Eq. (4.46)), the impact of the control point distribution on the error can be analyzed. Using the term ΔS, defined by Eq. (4.48), which is global and related to the total number of control points and the lattice spacing, this analysis can

be easily done. After several tests, it appears that in order to minimize the error, the control point distribution must be as symmetric and regular as possible. For the Couette flow problem, the discretization was achieved as follows: the inner and outer cylinders were discretized into circles with n and $2n$ points respectively, which correspond to a constant distance du between any two adjacent control points (see Fig. 4.14(a)). This way, the term ΔS is directly related to n, as the total number of control point m is proportional to n. In Fig. 4.14(b), error profiles with respect to parameter ΔS are plotted for four different lattice spacings and a Reynolds number of 10^{-1}. It can be observed that the optimal value of ΔS is located between 8 and 14. In that the term ΔS is related to n and cannot be freely chosen, only a finite number of values is possible. For example $\Delta S = 8.76$ corresponds to $n = 17$, $\Delta S = 13.96$ corresponds to $n = 16$, and no intermediate value exists. It is noteworthy that the error curves level off to constant values when $\Delta S \rightarrow 0$.
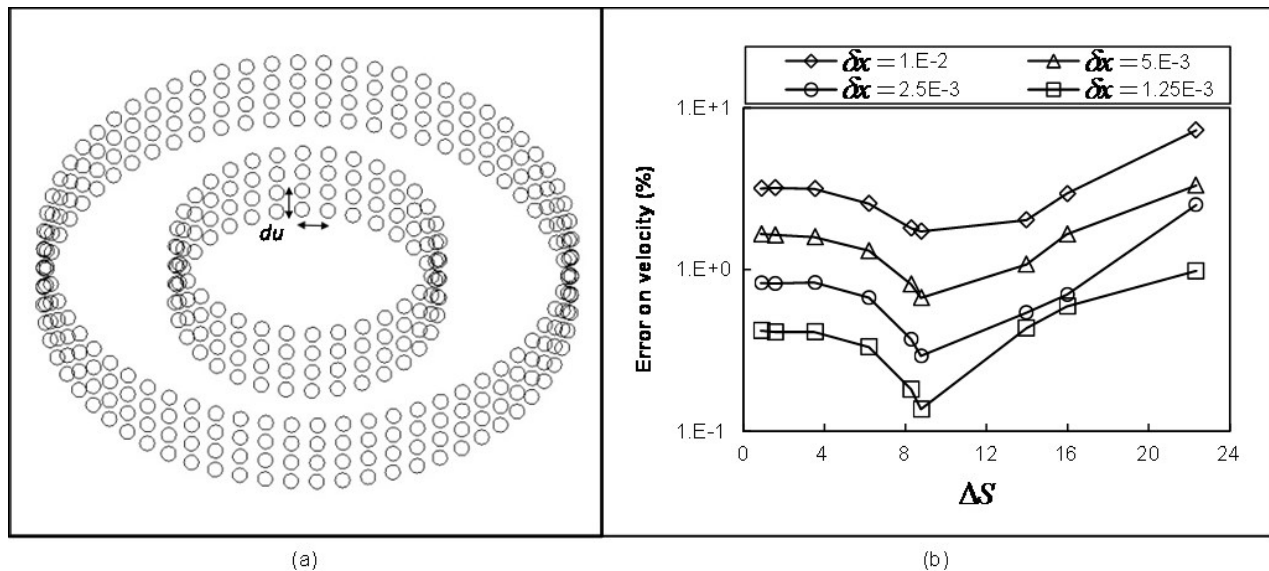
Figure 4.14: Impact of the control point distribution on the error for the IB-LBM

In order to help select the best value for ΔS, Fig. 4.15 demonstrates its impact on the order of convergence for the IB-LBM. The three selected values of ΔS are 6.21, 8.27 and 8.76 (corresponding to $n = 18$, 17 and 16) and the Reynolds number is 10^{-1}. It clearly appears that $\Delta S = 8.76$ yields the smallest error for all lattice spacings and the best order of convergence. This value was used for the mixing simulations carried out in this work.
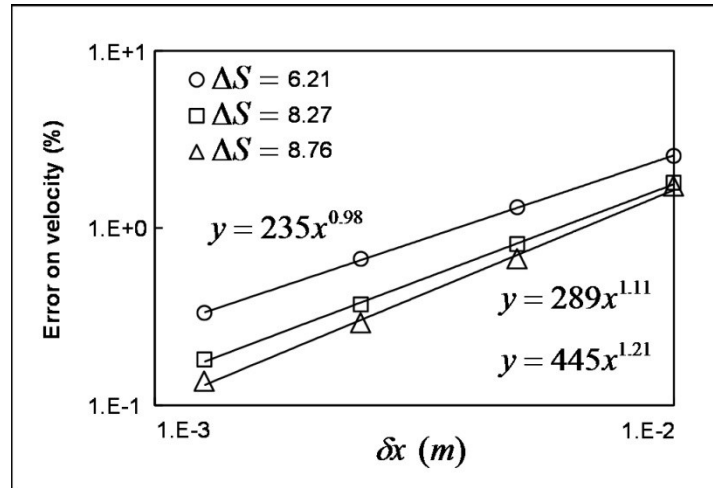
Figure 4.15: Impact of the number of control points on the order of convergence of the IB-LBM

4.2.6 Mixing simulations

On the basis of the findings of the previous section, the boundary condition parameters can now be chosen adequately for the simulation of fluid flow in industrial mixing systems. Two impellers are selected, the standard anchor and the Paravisc impeller (Ekato GmbH) (see Fig. 4.16), which are both used for the mixing of viscous fluids.
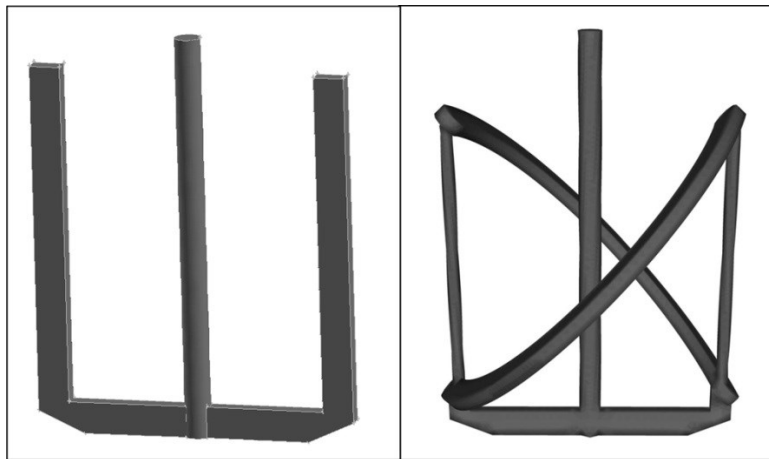
Figure 4.16: Geometry of the anchor impeller (left) and the Paravisc (Ekato GmbH) impeller (right).

For the mixing system with the anchor, the diameter of the tank is $D = 0.7\ m$, the diameter of the impeller is $d = 0.63\ m$ and the height of fluid is $h = 0.83\ m$. In the case of the Paravisc, the diameter of the tank is $D = 0.35\ m$, the diameter of the impeller is $d = 0.32\ m$ and the height of

fluid is $h = 0.4\,m$, as in Iranshahi *et al.* [41]. The simulated fluid is a Newtonian diluted corn syrup made up of 75% glucose. The corresponding density and viscosity are $\rho = 1400\,kg.m^{-3}$ and $\mu = 4\,Pa.s$. In both cases, the bottom of the tank is considered to be flat.

For a mixing system, the Reynolds number is defined as follows:

$$Re = \frac{\rho N d^2}{\mu} \tag{4.61}$$

where N is the rotational speed $(rev.s^{-1})$.

4.2.6.1 Lagrangian frame of reference

As mentioned in the introduction, the Lagrangian frame of reference is used, thus the impeller is consider to be fixed and the tank is rotating. This change of frame greatly simplifies the simulation process as it avoids simulating the motion of the impeller and thereby prevents the need to create new fluid lattices at each time iteration. In fact, the fluid domain is fixed in time so the discretization process (i.e. the selection of the fluid and solid lattice nodes) only has to be done once and the amount of data to be distributed amongst the processors is fixed. Such a configuration yields a steady state solution. Moreover, the simulations that were performed correspond to laminar regime with $Re \ll 1$. Under these conditions, the Coriolis force owing to the use of a rotating frame of reference is negligible.

4.2.6.2 Dimensionless numbers

The efficiency of a mixing system is determined by its capability to agitate or mix and the power consumption. In order to characterize the power consumption P (W) of a mixing system, the dimensionless power number N_p can be used:

$$N_p = \frac{P}{\rho N^3 d^5} \tag{4.62}$$

In the laminar regime, the dimensionless number K_p is preferred, given that its value is fixed for a given mixing system and is only related to its geometrical parameters. It is related to the power number N_p and Re:

$$K_p = N_p . Re \tag{4.63}$$

By injecting Eq. (4.62) into the previous definition, we obtain:

$$K_p = \frac{P}{\mu N^2 d^3} \tag{4.64}$$

As for the power consumption, it can be computed from the entire velocity field through the following equation [131]:

$$P = \int_\Omega \tau : \dot{\gamma} d\Omega \tag{4.65}$$

where τ is the stress tensor (Pa) and $\dot{\gamma}$ is the deformation rate tensor (s^{-1}).

In the case of a Newtonian fluid, Eq. (4.65) reduces to:

$$P = 2\mu \int_\Omega \dot{\gamma} : \dot{\gamma} d\Omega \tag{4.66}$$

where

$$\dot{\gamma}_{ij} = \frac{1}{2}\left(\frac{\delta u_i}{\delta x_j} + \frac{\delta u_j}{\delta x_i}\right), \quad \forall i,j = 1,2,3 \tag{4.67}$$

with $\vec{u} = (u_1, u_2, u_3)$ and $\vec{x} = (x_1, x_2, x_3)$.

There are two ways to compute the deformation rate within the context of the LBM, directly from the local populations or from the underlying spatial derivatives of the velocity, which in turn can be computed using finite difference formulas. As in the present implementation of the LBM the populations are not stored (see Section 4.2.3.1), the derivatives of the velocity are computed by a second-order centered formula:

$$\frac{\delta u_i}{\delta x_j} = \frac{u_i(\vec{x} + \vec{x}_j dx) - u_i(\vec{x} - \vec{x}_j dx)}{2dx} \tag{4.68}$$

where $\vec{x}_j$ refers to the unit vector associated to the coordinate j.

Near the solid parts one-sided forward and backward formulas are used:

$$\frac{\delta u_i}{\delta x_j} = (\mp)\frac{-3u_i(\vec{x}) + 4u_i(\vec{x} \mp \vec{x}_j dx) - u_i(\vec{x} \mp 2\vec{x}_j dx)}{2dx} \tag{4.69}$$

In order to determine the axial pumping capacity of the mixing system, the axial flow number N_q is used:

$$N_q = \frac{Q_z}{ND^3} \tag{4.70}$$

with the axial pumping rate Q_z given by:

$$Q_z = \frac{1}{h}\int_0^h \left(\int_S u_z^+ dS \right) dz = \frac{1}{h}\int_0^h \left(\int_S u_z^- dS \right) dz \tag{4.71}$$

where u_z^+ and u_z^- correspond respectively to the positive (0 when negative) and the negative (0 when positive) axial velocities, implying that the velocity field must conserve mass.

For the MBB and the EM, values of K_p and N_q were computed using the velocities at the fluid lattice nodes, as the solid lattice nodes represent the solid parts (see Section 4.2.6.4). In the case of the IB-LBM, as every lattice in the domain is fluid, all the lattices with a radius greater than the one of the tank were removed from the computation. Given that the volume of the impeller is small compared to that of the tank, the impact of the corresponding fluid lattice nodes in the computation of the dimensionless numbers is negligible.

4.2.6.3 Studied variables

In order to determine the impact of the boundary condition strategies on K_p and N_q, four different lattice spacings were considered. For the anchor, their values are:

$$\delta x \in [1;\ 0.5;\ 0.25;\ 0.125] * 10^{-2}m \tag{4.72}$$

For the Paravisc, they are given by:

$$\delta x \in [5;\ 2.5;\ 1.25;\ 0.625] * 10^{-3}m \tag{4.73}$$

The impact of the Reynolds number was also investigated. The selected Reynolds numbers belong to the laminar regime and their values are:

$$Re \in [10^{-3}; 10^{-2}; 10^{-1}] \tag{4.74}$$

The corresponding rotational speeds, which can be obtained from Eq. (4.61), are $[7.2 * 10^{-6}; 7.2 * 10^{-5}; 10^{-4}]$ for the anchor and $[2.8 * 10^{-5}; 2.8 * 10^{-4}; 2.8 * 10^{-3}]$ for the Paravisc.

The stopping condition defined by Eq. (4.56) was used, with a tolerance ε fixed at 10^{-4}. This value appears to be a good compromise between computational time and convergence.

4.2.6.4 Boundary conditions

As stated in Section 4.2.4, the different boundary condition strategies manage the solid parts differently. As for the modified bounce-back rule (MBB) and the extrapolation method (EM), the pre-processing step consists of determining which lattice nodes are solid inside the computational domain. For the tank, this step only requires selecting the lattices whose center has a r value larger than the radius of the tank. For the impeller, a volumetric mesh is used, so that the lattices with centers inside one element of the mesh are considered to be solid. With the EM strategy, a second operation is required, which computes the fraction Δ between the boundary lattices and the neighboring solid part. The fractions which are used to describe the tank are computed analytically, and the surface mesh obtained from the volumetric mesh is used to compute the fractions which describe the impeller. Following the conclusions of Section 4.2.5.2 for the EM, the ratio between the mesh size for the impeller and the lattice spacing was fixed to one, and the extrapolation parameters were computed as originally proposed by Guo *et al* [78]. In the present work, I-DEAS (Siemens) and Gambit (ANSYS) were used for the mesh generation of the impellers.

Contrary to the MBB and the EM, the immersed boundary-lattice Boltzmann method (IB-LBM) does not rely on the use of solid lattice nodes, so no search for such nodes is required. However, surface meshes are used to generate the control points needed by this method. Following the conclusions of Section 4.2.5.2, for every lattice spacing, the meshes were constructed by keeping the parameter ΔS at the optimal value ($\Delta S \approx 9$) found for the Couette flow. It is important to

mention that due to the use of the Lagrangian frame of reference, the control points representing the tank are each associated with a velocity that must converge to a value corresponding the kinematics of this tank. To limit the artificial interaction between the tank and the boundary of the computational domain, at least 20 lattices nodes were positioned along the gap between these two regions. This strategy was observed to yield values of K_p and N_q that do not depend on this gap. In the case of the Paravisc, the total number of fluid and solid lattice nodes for the three boundary condition strategies is summarized in Table 4.1.

Tableau 4.1: Total number of fluid (F) and solid (S) lattice nodes for the Paravisc impeller system.

Lattice spacing (mm)	5	2.5	1.25	0.625
MBB & EM	F: 293,450	F: 2,350,636	F: 18,810,322	F: 150,441,376
	S: 270,796	S: 1,952,250	S: 14,781,044	S: 114,987,750
IB-LBM	F: 877,286	F: 5,438,326	F: 37,907,606	F: 282,250,966

The fluid surface on top of the tank is approximated by a free surface boundary condition [58], which means that the surface is flat with a zero axial velocity. In the laminar regime, this approximation has been commonly used and has shown to be valid in various situations.

4.2.6.5 Results

4.2.6.5.1 Anchor mixer

The anchor impeller (Fig. 4.16) is one of the most basic impellers, as its geometry is quite simple. The associated flow is mainly rotational, indicating that the axial pumping is weak. Consequently, only the power consumption is considered in this study. The variations of the power number N_p with respect to the three values of the Reynolds number are plotted in Fig. 4.17 for (a) the MBB, (b) the EM and (c) the IB-LBM. From these three curves, it appears that, regardless of the discretization and the boundary condition strategy, the slope is equal to -1, which implies from Eq. (4.63) that K_p is constant.
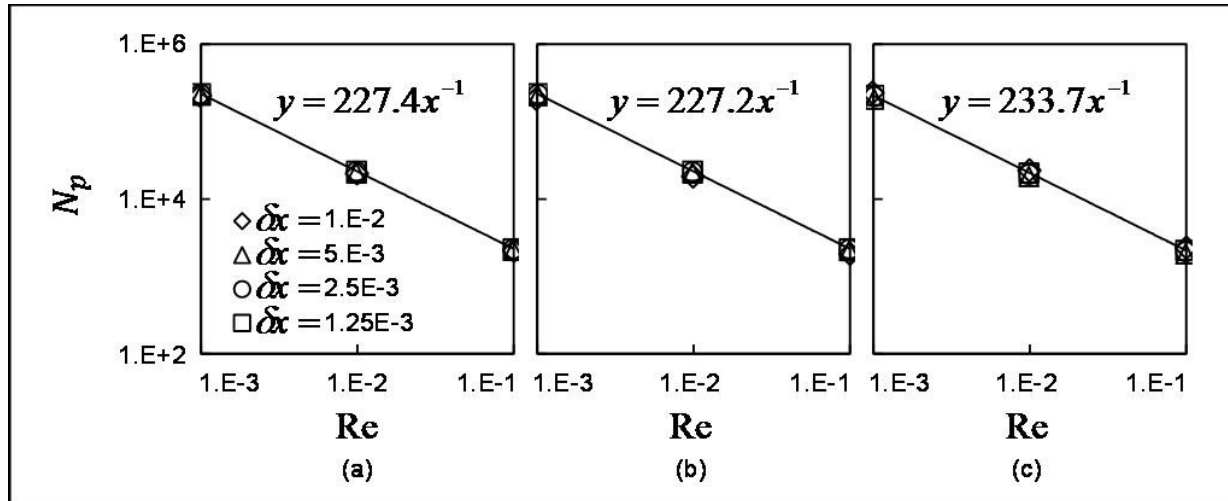
Figure 4.17: Power number for the anchor impeller system: (a) the MBB, (b) the EM and (c) the IB-LBM

In addition, it is essential to analyze the impact of the lattice spacing on the value of K_p. Fig. 4.18 shows its variations for the three different boundary condition strategies, at $Re = 10^{-1}$. The results are compared with experimental data from Foucault *et al.* [132] and a value obtained with the finite element method (FEM) using software POLY3D™. These FEM simulations used 193,000 linear $P_1^+ - P_1$ tetrahedral (MINI) elements, corresponding to a total number of 118,000 velocity-pressure equations. The underlying linear systems were solved by means of a Krylov-based Uzawa solver. First, it can be noticed that the results obtained with all the boundary conditions strategies converge to values close to experimental data and the FEM result when the lattice spacing δx is decreased. Second, the results with the MBB and the EM are close and the convergence rate is good with variations under 2% when δx goes from $1.25 * 10^{-3}$ to $2.5 * 10^{-3}$. The convergence profile is also similar for the IB-LBM but the values of K_p remain less than 10% lower. This indicates that despite the fact that convergence is observed, this boundary condition strategy is not as accurate as the MBB and the EM. The discrepancy can be explained by the high error in velocity near the solid parts as discussed in Section 4.2.5.1.2.
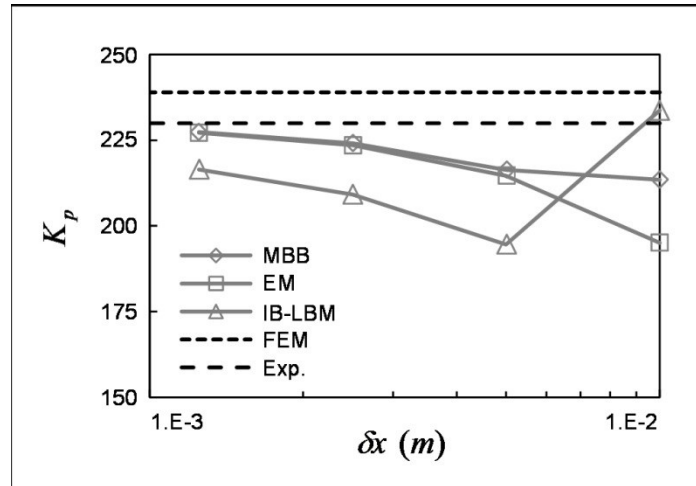
Figure 4.18: Convergence of Kp with respect to the lattice spacing for the anchor impeller system

4.2.6.5.2 Paravisc mixer

The Paravisc impeller (Fig. 4.16) can be considered as an improved anchor, in which the vertical arms have been twisted to improve the axial pumping rate, in a similar way as the helical ribbon impeller. For this mixing configuration, values of K_p and N_q obtained with the three boundary condition strategies are compared to results available in the literature. The experimental data come from Delaplace *et al.* [133] and the FEM results are from Iranshahi *et al.* [41]. In the latter work, 130,000 linear $P_1^+ - P_0$ tetrahedral elements were used, corresponding to a total number of 940,000 velocity-pressure equations. The underlying linear systems were solved by means of a Krylov-based Uzawa solver.

The variations of the power draw, at $Re = 10^{-1}$, with respect to the lattice spacing is plotted in Fig. 4.19. As for the anchor impeller, the results exhibit a good agreement with the experimental data and the FEM results. Once again, the results with the MBB and the EM are close and the convergence rate is good, as the K_p values between the two smallest lattice spacings differ by less than 2%. With the IB-LBM, the convergence profile is different and, surprisingly enough, the variation of the K_p values are negligible for the three smallest lattice spacings. As will be seen next, this behavior does not hold for the axial flow number.
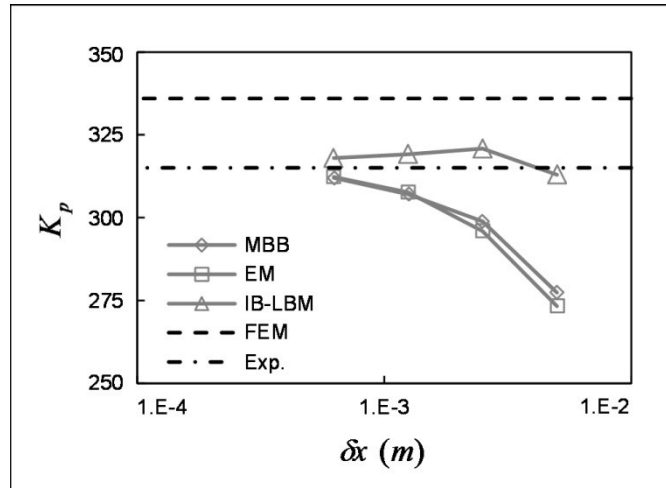
Figure 4.19: Convergence of Kp with respect to the lattice spacing for the Paravisc impeller system
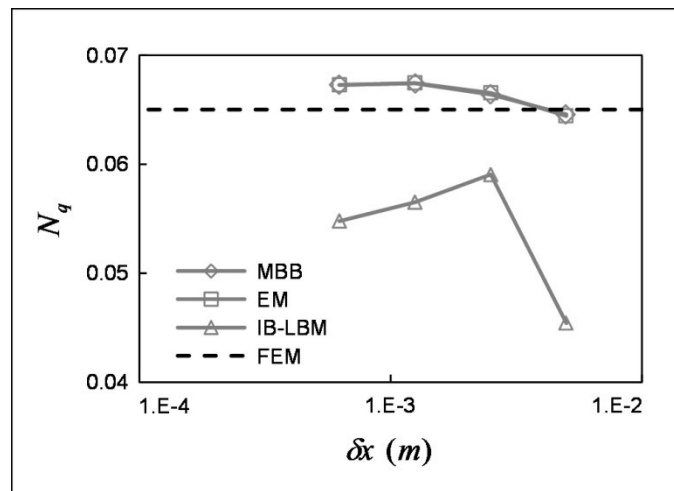
Figure 4.20: Convergence of the axial flow number N_q with respect to the lattice spacing for the Paravisc impeller system

The variations of the axial flow number N_q with respect to the lattice spacing are plotted in Fig. 4.20. The results with the MBB and the EM are similar and agree well with the FEM results. The influence of the lattice size is observed to be rather small with results between the two smallest lattice spacings that differ by only 0.2%. This difference can be explained by the fact that only the axial component of the velocity is used, which means that the error on the other components does not appear in the axial flow number. As for the IB-LBM, the values obtained are much lower than those of the other two approaches and the FEM. In addition, the variations of the axial

flow number with respect to the lattice spacing are larger, which is due to the fact that this boundary condition strategy cannot accurately model impeller-wall interactions for such a small wall clearance. It can be inferred from Figs. 4.19 and 4.20 that a converged value of K_p does not guarantee that the flow field is predicated accurately, which shows that N_q is more sensitive than K_p to local errors on velocity. For instance, Fig. 4.21 presents contours of the norm of the velocity on a horizontal cross-section at $z = 0.4\ m$, for $Re = 10^{-1}$ and $\delta x = 10^{-2} m$, in the case of the three different boundary condition strategies. Figs. 4.21(a) and 4.21(b) confirm that the flow fields obtained with the MBB and the EM are similar, as no significant differences can be observed on the norm of the velocity. However, Fig. 4.21(c) clearly shows that the flow around the impeller is not as accurately predicted by the IB-LBM. In fact, even if the flow is globally well described with this approach, the contours reveal that this strategy can overestimate the local velocity in a specific area (e.g. upper left part of the figure) while it underestimates it in other locations (e.g lower right part of the figure). These erroneous velocities observed in the zones of the impeller may result in streamlines going through it.
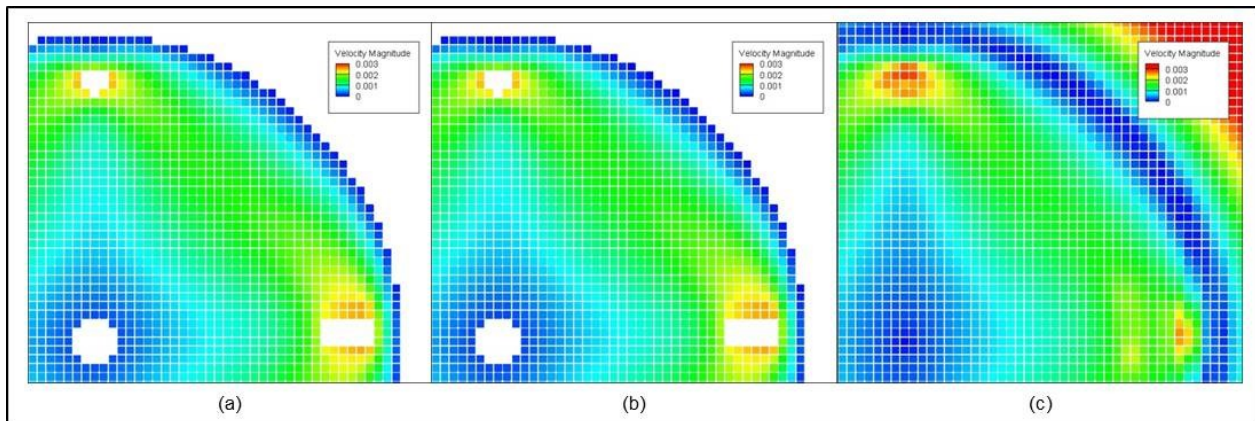
Figure 4.21: Contours of the norm of the velocity on a horizontal cross-section with (a) the MBB, (b) the EM and the (c) IB-LBM. ($z = 0.4\ m$, $Re = 10^{-1}$ and $\delta x = 10^{-2} m$)

4.2.7 Parallel performance and memory usage

As specified in Section 4.2.4, the different boundary condition strategies can perturb the intrinsically high parallel efficiency of the lattice Boltzmann method. In the case of the modified bounce-back rule (MBB), as with the original half way bounce-back rule, the efficiency of the LBM scheme is conserved due to the locality of the operations inherent to this boundary

condition strategy. Unfortunately, this is not true for the other strategies, as they rely on interpolations or extrapolations that require non-local computations.

For the extrapolation method (EM), as previously discussed in Section 4.2.4.2, the computations only require information from the neighboring lattices used for the propagation step. Consequently, this strategy does not require modifications to the communication scheme between the processors; it thus conserves the parallel efficiency of the standard LBM. As the extrapolation computations are simple, the workload is not perturbed. The only real issue with this boundary condition strategy is the computation of fractions for solid parts with complex shapes. In this work, the surfaces of solid parts are described using meshes, which imply matching the boundary lattices with the corresponding mesh elements using a search algorithm. However, since the Lagrangian frame of reference is used, the location of these solid parts is fixed and the fractions are computed only once as a pre-processing operation.

The immersed boundary-lattice Boltzmann method (IB-LBM) strategy is completely different since it consists of a global approach. As a result, in order to compute the required body force, a system of equations needs to be solved. Although the size of the system is proportional to the total number of control points, which is small compared to the total number of lattice nodes, the computational time associated to its solution can be important and increase the workload. Furthermore, the system of equations needs to be solved at each time step, as the right-hand-side is a function of the current flow field. Once again, due to the use of the Lagrangian frame of reference, the process is simplified as the position of the control points is fixed, which avoids recomputing the matrix at each time step. Unfortunately, the solution of the system does not only increase the computational time, it also needs a more complex communication scheme between the processors, which must be executed at each time step. First, the right-hand-side needs to be built by gathering information. Second, the solution of the linear system (i.e. the body force) needs to be distributed among the processors. Finally, the last communication step concerns the summation of corrections on the lattice nodes near the communication zones (see Section 4.2.4.3). It is also important to mention that the solution of the system of equations is not parallel in our implementation, so only one processor is used during this step. This leads to a slight decrease of the parallel efficiency of the IB-LBM.

Tableau 4.2: Characteristics of the supercomputer used for the simulation.

Characteristics	Mammouth
Number of nodes	576
Type of node	One Intel Xeon 3.6 GHz 64-bit twin-core processor
Total number of core	1152
Memory per node	8 GB
Total available memory	4.5 TB
Network	Infiniband DDR (16 Gb/s)
Peak performance	9 Tflops

To analyze the impact of the three boundary condition strategies on the workload, the computational times associated with the simulation of the Paravisc impeller system were evaluated. The computations were performed on a super computer (Calcul Quebec Mammouth-parallel supercomputer), the characteristics of which are summarized in Table 4.2. The average performance is on the order of 100 million lattice-site updates per second.
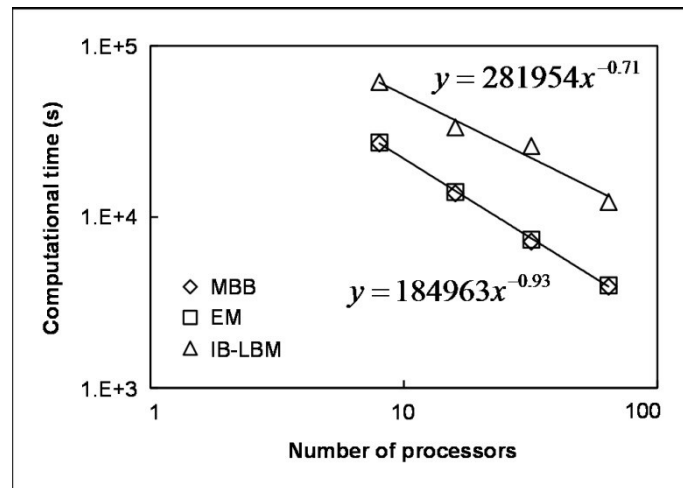
Figure 4.22: Graph of the computational time vs the number of processors

The Reynolds number was fixed at $Re = 10^{-3}$, the selected lattice spacing was $\delta x = 1.25 *$ $10^{-3}\ m$ and the tolerance ε was fixed at 10^{-4}. The computational times associated with these three boundary condition strategies are plotted with respect to the number of processors in Fig. 4.22. From these curves, it appears that the computational times with the MBB and the EM are similar, which means that the cost associated with the extrapolation computations is negligible, even if these computations are not fully local. The slope of the curve is close to -1, indicating a linear speed up. As for the IB-LBM, the computational times are higher. This is not surprising since this strategy needs to solve a system of equations in addition to performing the classical collision and propagation steps. The slope of the curve is also modified, which implies that the parallel efficiency is deteriorated by the solution of this system and supplementary inter-process communications.

Tableau 4.3: Memory usage for the three boundary conditions strategies.

Lattice spacing (mm)	5	2.5	1.25	0.625
MBB (reference)	26.32 MB	204.3 MB	1.61 GB	12.77 GB
EM (scheme)	26.32 MB	204.3 MB	1.61 GB	12.77 GB
EM (BC)	1.328 MB (+5%)	5.418 MB (+2.6%)	21.73 MB (+1.3%)	85.34 MB (+0.7%)
EM (total)	27.65 MB	209.7 MB	1.632 GB	12.85 GB
IB-LBM (scheme)	54.39 MB (+107%)	337.2 MB (+65%)	2.35 GB (+46%)	17.5 GB (+37%)
IB-LBM (BC)	0.266 MB (+1%)	0.684 MB (+0.3%)	2.826 MB (+0.2%)	11.29 MB (+0.08%)
IB-LBM (total)	54.66 MB	337.9 MB	2.353 GB	17.51 GB

It is also important to examine the impact of the boundary condition strategies on the memory usage. Once again, the MBB does not require any modification, so it is considered as the reference. The EM requires the computation of fractions that need to be stored. The supplementary memory required is then proportional to the total number of pairs of solid-fluid

lattice nodes. The IB-LBM is based on a completely different approach, hence the memory usage is different. First, the system of equations and the control point coordinates need to be stored. Given that the system matrix is sparse, the Compressed Sparse Row (CSR) format [134] is used here to reduce memory usage. Second, because all the lattice nodes are fluid, the required memory is increased in comparison to the MBB and the EM. This supplementary memory corresponds to the storage of the velocity and the density information on those lattices that are considered solid when using the MBB or the EM. More memory is also required because of the increase of the size of the domain to reduce the interactions between the control points and its boundary (see Section 4.2.6.4). Table 4.3 sums up the memory usage associated with the simulation of the fluid flow in the Paravisc impeller system for four different lattice spacings. In that the MBB is considered as the reference, the memory usage for the EM and the IB-LBM is divided into two parts: the storage of the variables for the regular LBM scheme (referred to as scheme) and the storage associated with the boundary condition strategy (referred to as BC). According to this table, it seems that the supplementary memory required by the boundary condition strategies (BC) is negligible for both the EM (from 0.7% to 5%) and the IB-LBM (from 0.08% to 1%). This result can be explained by the fact the boundary conditions are related to surfaces, so the amount of information is negligible compared to that required for the entire volume. Obviously, this conclusion is limited to mixing systems with a large volume to surface ratio. The use of the IB-LBM remarkably increases the memory required for the scheme, from 37% (smallest lattice size) to 107% (largest lattice size). This is due to the increase in the size of the domain to reduce the interactions between the control points and its boundary (see Section 4.2.6.4).

4.2.8 Conclusion

The objective of this work was to characterize the suitability of three different strategies for imposing boundary conditions in the lattice Boltzmann method for the 3D simulation of viscous mixing flows. The three selected strategies were the modified bounce-back (MBB) rule, the extrapolation method (EM) and the immersed boundary-lattice Boltzmann method (IB-LBM).

Thanks to the simulation of the Couette flow problem, the impact of the three strategies on the spatial convergence was analyzed. It was shown that only the EM is capable of conserving the second order accuracy of the LBM while yielding the most accurate results. The deterioration

observed with the other strategies was also pointed out. The error with the MBB was related to oscillations in the entire computational domain, and the error with the IB-LBM appears to be due to a high error on the velocity close to the solid parts. The parameters of the EM and the IB-LBM were also investigated. For the EM, it appears that the original formulation of the extrapolation parameters was the most stable choice. Regarding the computation of the fractions, the description of the solid part surfaces by meshes was tested and showed that, in order to conserve the second order accuracy of the scheme, the ratio between the lattice spacing and the mesh size must be constant. As for the IB-LBM, it was shown that an optimal value of ΔS exists for the distribution of control points.

The boundary condition strategies were also compared on the simulation of anchor and Paravisc impeller systems (Section 4.2.6). Using the Lagrangian frame of reference, the accuracy of these three boundary condition strategies was quantified by means of the power constant K_p and the axial flow number N_q. It was shown that the LBM results are in accord with the experimental data and finite element simulation results, and that, surprisingly enough, the MBB provides a reliable accuracy despite its simplicity. In fact, the results and the convergence profiles of the MBB and the EM were similar on the basis of both dimensionless numbers. With the IB-LBM, even if the results were not so far from the experimental data and the finite element simulation results, the predicted values of K_p and N_q and their related convergence, with respect to lattice spacing, were different compared to those of the other two boundary condition strategies. This indicates that the IB-LBM yields a somewhat different flow field. This was further confirmed by comparing the contours of the norm of the velocity on a cross-section obtained with the three different approaches.

Finally, the impact of the boundary condition strategies on the workload and memory usage was analyzed for the Paravisc impeller system (Section 4.2.7). It appears that the MBB and the EM both conserve the high parallel efficiency of the standard LBM. Moreover, the impact of the extrapolation computations on the total simulation time is small. For the IB-LBM, as it is based on a global approach and requires solving a system of equations, the computational time and the workload are both increased, so the parallel efficiency is reduced. Lastly, even though the EM and the IB-LBM require the storing of additional data, no significant impact was noticed as

regards the memory usage. In summary, this work showed that the MBB is a good compromise for the simulation of viscous mixing flows.

4.2.9 Acknowledgments

CHAPITRE 5   ÉTUDE DE LA PRÉCISION DE LA LBM DANS LE CAS DE GÉOMÉTRIES COMPLEXES

5.1   Présentation du deuxième article

Soumis à *International Journal for Numerical Methods in Fluids* le 23 Novembre 2012.

Auteurs : Vincent Stobiac, Philippe Tanguy, François Bertrand.

Cet article traite de l'applicabilité de la méthode d'extrapolation pour la simulation du mélange visqueux avec la méthode de Boltzmann sur réseau. Suite à la comparaison des stratégies d'imposition de conditions aux limites présentée dans l'article 1, il apparait que la méthode d'extrapolation permet de traiter plus précisément les géométries complexes, et est donc mieux adaptée pour la simulation d'écoulements dans des mélangeurs raclants. Dans cet article, la qualité des résultats est caractérisée sur les prédictions de consommation de puissance et de capacité de pompage au sein du système de mélange Maxblend. Ce mélangeur a été choisi car il présente de bonnes performances sur une large gamme de nombre de Reynolds. Tout d'abord, la sensibilité de la précision de la LBM par rapport aux conditions aux limites est étudiée sur l'écoulement de Couette cylindrique. Il ressort qu'une petite modification des conditions aux limites peut largement réduire la précision des prédictions de taux de cisaillement et de consommation de puissance. Ensuite, l'écoulement dans le Maxblend est simulé à l'aide d'un code LBM massivement parallèle. Pour la configuration sans contre-pale, les prédictions de consommations de puissance et de création de pompage sont en accord avec les données disponibles dans la littérature. En complément, l'impact de l'espacement entre la pale et le fond de la cuve a aussi été étudié, montrant que la valeur standard n'est pas optimale en régime transitoire. Finalement, pour la configuration la plus complexe, c'est-à-dire avec contre-pale, les simulations montrent que des perturbations apparaissent autour de la pale. Au final, les résultats cet article montrent que la méthode de Boltzmann sur réseau, couplée avec la méthode d'extrapolation, est un outil efficace pour la simulation d'écoulements visqueux dans des mélangeurs raclants.

5.2 A thorough investigation of the accuracy of the extrapolation method for the lattice Boltzmann simulation of viscous fluid flow in a Maxblend impeller system

5.2.1 Summary

This paper offers a thorough assessment on the performance of the extrapolation method for the lattice Boltzmann simulation of viscous mixing flows. This method appears to be well-suited for the treatment of the complex boundary conditions found in various mixing systems. Here, the ability to simulate accurate power consumption and pumping capacity is evaluated on several configurations of the Maxblend mixing system, which has proven efficient in a wide range of applications. First, the impact of the boundary conditions on the spatial convergence of the lattice Boltzmann method (LBM) is determined on the 3D Couette flow, clearly showing that small modifications of the boundary conditions may reduce the accuracy of the predicted shear rate and power. Second, a parallel LBM scheme was used to simulate fluid flow within a Maxblend mixing system. For the unbaffled configuration, the simulated power consumption and the pumping capacity are observed to be in good agreement with experimental data and finite element simulation results. The effect of the bottom clearance is also successfully evaluated, suggesting that the standard bottom clearance is not optimum in the transitional regime. Lastly, results for the most geometrically complex case (baffled configuration) indicate that the power consumption is affected by numerical perturbations appearing around the moving impeller. Overall, these results show that, when combined with the extrapolation method for the treatment of boundary conditions, the LBM is an efficient tool for the investigation of viscous flow in mixers of industrial relevance.

5.2.2 Introduction

The lattice Boltzmann method (LBM) is a powerful numerical method that has been successfully applied for the simulation of various industrial flows, such as those in catalytic converters [7, 135], stirred tank reactors [27, 98] and static mixers [136, 137]. This method differs from the classical CFD methods, the finite element method (FEM) and the finite volume method (FVM), in that the solution obtained for the Navier-Stokes equations uses the mesoscopic scale rather than the macroscopic scale. Owing to this change of scale, the modeling of several hydrodynamic

phenomena, such as those induced by turbulence [86, 116, 138] or complex rheology [16, 54, 115], is simplified. The LBM also has a linear constitutive equation (the lattice Boltzmann equation) both simple and local. When applied on a structured Cartesian grid, such advantages give the LBM its highly intrinsic parallel performance, which has been favourably used to reduce simulation costs for geometrically complex flow problems involving, for instance, porous media [3, 110, 115] or solid-fluid suspensions [72, 111, 139].

Inversely, the major drawback of the LBM is in the definition of macroscopic boundary conditions, which are crucial for complex geometries. While the so-called modified bounce-back rule [72] has been commonly considered to impose a non-zero velocity along curved boundaries, its use is known to decrease the accuracy of the LBM scheme [73, 74, 140]. Lately, alternate strategies have been proposed to reduce these inaccuracies, namely the extrapolation or interpolation methods [76-79] and the immersed boundary methods [16, 81, 83].

Simulation of mixing in stirred tanks is a challenging problem of industrial relevance, the results of which can serve for process design and optimization. The geometries of stirred tanks are highly complex and present several difficulties, such as the motion of the impeller or the small gap between this impeller and the tank wall. In this context, the LBM has been successfully used for the simulation of turbulent mixing flows [27, 54, 86, 117, 141, 142]. In mixing systems comprised of a Rushton turbine, such simulations have permitted to investigate flow fields in the vicinity of the impeller [27, 54, 86, 117, 141, 142], as well as evaluate the turbulent kinetic energy [54, 86, 117, 141, 142], the energy dissipation rate [86, 117], the apparent viscosity [54] and the volume of caverns in the case of Bingham fluids [27].

In contrast to the mixing occurring inside the vortices of turbulent flows, the mixing in viscous flow systems is driven by the shear-induced stretching, folding and breaking mechanisms of the fluid streams generated by the close-clearance impeller. The complexity of the geometry is therefore increased by the presence of a small wall clearance, within which it becomes essential to accurately capture the flow. We believe the difficulty in imposing accurate boundary conditions is one of the reasons why the LBM has rarely been used in this context. In our previous study [140], we showed that, in the case of a fixed geometry, the different boundary condition strategies investigated, let alone the modified bounce-back [72], the extrapolation [78] and the immersed boundary [83] methods, are not all equivalent in terms of accuracy. In

particular, the simulation of a Couette flow showed that the extrapolation method is the only strategy that preserves the second-order accuracy of the LBM. When applied to mixing systems, the modified bounce-back rule and the extrapolation method (EM) were observed to be potentially good choices for the prediction of power consumption and pumping capacity in the case of anchor and Paravisc impeller systems. For these reasons and considering that the slightly larger cost of the extrapolation method with respect to the modified bounce-back rule is compensated by the gain in accuracy, the former was used in this work.

This investigation provides a thorough assessment of the accuracy of the LBM and EM combination for the simulation of geometrically complex mixing flows. The emphasis is put on the simulated power consumption and pumping capacity, which are two important characteristic numbers for mixer comparison. The Maxblend impeller (Sumitomo Heavy Industries, Japan) has been selected for this study, as it has been observed to be an efficient mixer in various applications [35]. Several experimental and numerical investigations on design parameters [13, 33, 36, 143] are available in the literature and will be used to assess our results. We have chosen to focus on the impact on power consumption and pumping capacity of a small variation of the bottom clearance. The procedure for simulating the motion of the impeller is also investigated. To our knowledge, no extended analysis for such complex 3D flows have yet been reported. Moreover, the conclusions of the present study are not limited to mixing flows and may be applicable to other types of geometrically complex flow situations.

The organization of the paper is as follows. In Section 5.2.3, the LBM is revisited including the specifications of the implementation used in this work. In Section 5.2.4, the three-dimensional Couette flow problem is simulated to verify the spatial convergence of the scheme as regards the shear rate and the power. The impacts of the boundary conditions are also investigated. In Section 5.2.5, the lattice Boltzmann scheme is used to simulate the hydrodynamics of the Maxblend impeller. First, using a Lagrangian frame of reference, the performance of the unbaffled mixing system is characterized for several values of the bottom clearance. Second, the accuracy of the predicted power consumption is studied for the baffled configuration. Concluding remarks are given in Section 5.2.6.

5.2.3 The lattice Boltzmann method

Only a brief presentation of the method is provided here and the reader is referred to [58, 144] for detailed explanations. Contrary to the classical CFD tools, the LBM is based on the kinetic theory of gas, situated at the mesoscopic scale. The solution of the Navier-Stokes equations is then recovered from the solution of the Boltzmann equation using populations of particles. These populations propagate and collide along the bonds of a lattice grid and their motions are governed by a simple recurrence equation. The main advantages of the resulting scheme are the linearity and simplicity of the constitutive equation, giving the LBM its high parallel performance.

First we consider the population $f_k(\vec{x}, t)$ at position $\vec{x}$, with velocity $\vec{e}_k$, at time t, so that in every lattice, macroscopic variables such as the density ρ and the velocity $\vec{u}$ can be easily recovered as [65]:

$$\rho(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t) \tag{5.1}$$

$$\rho_0 \vec{u}(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t)\, \vec{e}_k + \frac{\delta t}{2}\, \vec{g}(\vec{x}, t) \tag{5.2}$$

where q is the total number of populations per lattice, ρ_0 is the mean density, $\vec{g}(\vec{x}, t)$ is a body force density and δt is the time step. In the present work, the 15-population D3Q15 lattice [63] is chosen since preliminary results demonstrated that, compared to lattices with more populations (19 and 27), the accuracy is comparable and the computational time is reduced.

The lattice Boltzmann equation, coupled with the BGK collision operator [60, 63], is defined as follows:

$$f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) - f_k(\vec{x}, t) = -\frac{1}{\tau}\left[f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t) \right] + \delta t\, G_k(\vec{x}, t) \tag{5.3}$$

where the forcing term G_k is given by [65]

$$G_k(\vec{x}, t) = \left(1 - \frac{1}{2\tau}\right) \omega_k \left[\frac{\vec{e}_k - \vec{u}}{c_s^2} + \frac{(\vec{e}_k . \vec{u})}{c_s^4} \vec{e}_k \right] . \vec{g}(\vec{x}, t) \tag{5.4}$$

and the equilibrium population is defined as

$$f_k^{(eq)}(\vec{x}, t) = \omega_k \left[\rho + \rho_0 \left(\frac{\vec{e}_k \cdot \vec{u}}{c_s^2} + \frac{(\vec{e}_k \cdot \vec{u})^2}{2c_s^4} - \frac{\vec{u} \cdot \vec{u}}{2c_s^2} \right) \right] \tag{5.5}$$

Where δx is the lattice spacing, τ is the relaxation parameter, $c_s = \frac{1}{\sqrt{3}} \frac{\delta x}{\delta t}$ is the speed of sound, and the weights ω_k are, for the D3Q15 lattice, $\frac{2}{9}$ if $k = 0$, $\frac{1}{9}$ if $k = 1,6$ and $\frac{1}{72}$ if $k = 7,14$.

The relaxation parameter τ is related to the fluid viscosity μ by the following relation:

$$\tau = \frac{\mu}{\rho \delta t c_s^2} + \frac{1}{2} \tag{5.6}$$

The solution of the Navier-Stokes equations is recovered under the hypotheses of small Mach $\left(Ma = \frac{\|\vec{u}\|}{c_s} \right)$ and small Knudsen $\left(Kn = \frac{\mu}{\rho L c_s} \right)$ numbers, where L is a characteristic length. In the case of diffusive scaling (i.e. $\delta t \propto \delta x^2$), the resulting explicit scheme has been proven to be second order accurate in space [121, 144, 145] in the case of a periodic computational domain. However, the accuracy of the scheme can be largely affected by the boundary conditions.

5.2.3.1 Boundary conditions

It is noteworthy that the LBM scheme defined by Eq. (5.3) is only valid for a lattice node $\vec{x}$ situated inside the computational domain. As a result, it must be completed by boundary conditions at the boundary of the domain. As mentioned in the introduction, the fact that the primary variable f_k is mesoscopic is a drawback as regards the imposition of macroscopic boundary conditions on velocity. However, in the case of an exact discretization (i.e. all boundaries are situated precisely on lattice nodes or half a grid spacing away), several simple rules may be applied to missing populations in order to model boundary conditions. For example, Dirichlet boundary conditions on velocity can be defined by the so-called modified bounce-back rule [72]. In the same manner, free slip boundary conditions [58] may be used to model surfaces without friction. These boundary condition strategies can conserve the second order accuracy of the LBM. However, in the case of curved boundaries, such strategies are known to reduce the accuracy to the first order [73, 74].

For the purposes of this work, in order to accurately describe the geometry of the mixing system, all boundary conditions except those at the free surface are imposed with the extrapolation method (EM) [78]. The second order accuracy is then conserved [74, 78, 140] and the exact position of the boundaries is computed and stored. To do so, this boundary condition strategy requires the computation of the fraction Δ representing the distance between the fluid node and the boundary (see Fig. 5.1). The fraction is computed as $\Delta = \frac{|\vec{x}_f - \vec{x}_b|}{|\vec{x}_f - \vec{x}_w|}$, where $\vec{x}_w$ and $\vec{x}_f$ correspond respectively to the position of the solid and fluid nodes, and $\vec{x}_b$ is the intersection between the actual boundary and the line joining $\vec{x}_w$ and $\vec{x}_f$. Based on the decomposition of the populations into equilibrium and non-equilibrium parts, i.e. $f_k(\vec{x}, t) = f_k^{(eq)}(\vec{x}, t) + f_k^{(neq)}(\vec{x}, t)$, the EM uses the fraction Δ to extrapolate the velocity and the non-equilibrium populations at the solid node $\vec{x}_w$.
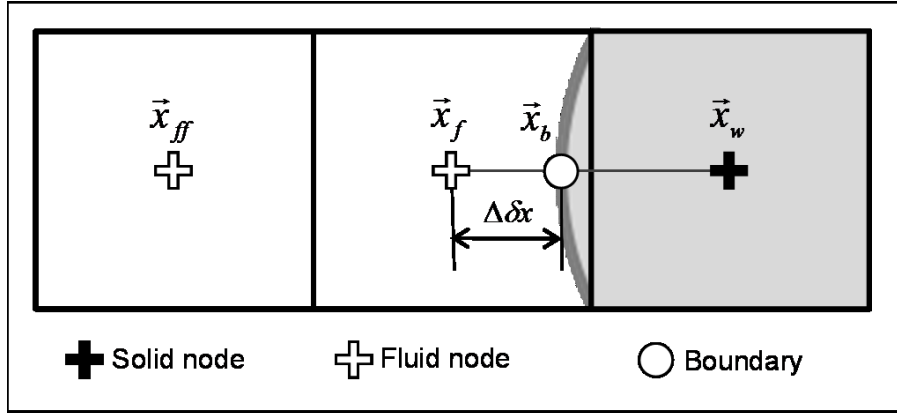
Figure 5.1: Distance to the boundary with the extrapolation method (EM).

The unknown populations at the first fluid node $\vec{x}_f$ are computed as follows:

$$f_k(\vec{x}_f, t + \delta t) = f_k^{(eq)}(\vec{x}_w, t) + \left(1 - \frac{1}{\tau}\right) f_k^{(neq)}(\vec{x}_w, t) \tag{5.7}$$

The equilibrium part is computed with Eq. (5.5), where the density $\rho(\vec{x}_w, t)$ is approximated by $\rho(\vec{x}_f, t)$, and the velocity $\vec{u}_w = \vec{u}(\vec{x}_w, t)$ at the solid node is determined by the following extrapolation procedure:

$$\vec{u}_w = \gamma_0 \vec{u}_b + \gamma_1 \vec{u}_f + \gamma_2 \vec{u}_{ff} \tag{5.8}$$

where $\vec{u}_b$, $\vec{u}_f$ and $\vec{u}_{ff}$ correspond to the velocity at nodes $\vec{x}_b$, $\vec{x}_f$ and $\vec{x}_{ff}$, respectively (see Fig. 5.1). The formulas for the extrapolation parameters γ_i are given in Table 5.1.

Tableau 5.1: Formulas for the parameters of the extrapolation method (EM).

	γ_0	γ_1	γ_2	β
$\Delta < 0.75$	$\dfrac{3-\Delta}{1+\Delta}$	$\Delta - 1$	$-\dfrac{(1-\Delta)^2}{(1+\Delta)}$	Δ
$\Delta \geq 0.75$	$\dfrac{1}{\Delta}$	$\dfrac{\Delta - 1}{\Delta}$	0	1

Next, the non-equilibrium part of Eq. (5.7) is directly extrapolated from the neighboring nodes as

$$f_k^{(neq)}(\vec{x}_w, t) = \beta f_k^{(neq)}(\vec{x}_f, t) + (1 - \beta)f_k^{(neq)}(\vec{x}_{ff}, t) \tag{5.9}$$

where the extrapolation parameter β is defined in Table 5.1.

It is important to mention that Eqs. (5.8) and (5.9), which describe the boundary condition strategy, are only valid if the lattice node $\vec{x}_{ff}$ is fluid. Otherwise, we propose to impose $\vec{u}_w = \vec{u}_b$ and $f_k^{(neq)}(\vec{x}_w, t) = f_k^{(neq)}(\vec{x}_f, t)$.

5.2.3.2 Power computation

Independent of the numerical method used, the power may be obtained in two distinct manners. First, it can be computed as a volume integral of the viscous dissipation, $P = \int_\Omega \sigma : \dot{\gamma} d\Omega$, where Ω denotes the computational domain and σ and $\dot{\gamma}$ are the stress tensor and the shear rate tensor, respectively. In the case of a Newtonian fluid, this formula reduces to

$$P = 2\mu \int_\Omega \dot{\gamma} : \dot{\gamma} d\Omega \tag{5.10}$$

With the LBM, the shear rate tensor can be computed from the velocity field with a second-order centered difference formula, but it can also be computed directly from the populations inside a lattice. The latter computation is local and expressed for the ij component of $\dot{\gamma}$ by [62, 89]:

$$\dot{\gamma}_{ij} = -\frac{1}{2\tau\rho_0 c_s^2 \delta t} \sum_{k=0}^{n-1} \left(\vec{e}_{ki}\vec{e}_{kj} - \frac{\delta_{ij}}{D} \vec{e}_k \cdot \vec{e}_k \right) f_k^{(neq)} \tag{5.11}$$

where D is the dimension of the problem (3 in this work) and δ_{ij} is the Kronecker delta function. In this work, the shear rate is computed from the populations in all cases since our tests showed that the difference between the two approaches is negligible.

Second, the power can be computed as a surface integral of the force moment acting at the boundary, the torque, times the angular velocity ω:

$$P = \omega \int_{\Gamma} (\vec{x} - \vec{x}_c) \times \vec{F} d\Gamma \tag{5.12}$$

where $\vec{x}_c$ is the center of gravity, Γ is the boundary of the domain and $\vec{F}$ is the force per unit surface acting at the boundary. With the LBM, this force can be readily computed from the populations with the so-called momentum exchange algorithm [72]. More precisely, for every direction k involving a boundary condition, the force can be approximated by [72, 89, 146]

$$\vec{F}_k = \frac{\delta x^3}{\delta t} \left(f_k(\vec{x}, t_+) + f_{k'}(\vec{x}, t + \delta t) \right) \vec{e}_k \tag{5.13}$$

where t_+ refers to the post-collision time (after a collision but before the next propagation step) and k' is the direction opposite of k.

The important fact here is that the simulation itself is not affected by the approach used to compute the power. In other words, this computation is similar to a post-processing step. Therefore, two different values of the power can be obtained. It can already be inferred that, since the evaluation of $\vec{F}_k$ in Eq. (5.13) is less expensive than that of $\dot{\gamma}_{ij}$ in Eq. (5.11), and can be done during the computation of the boundary conditions, the method based on the torque requires less computational time than that based on the shear rate. It is then important to determine if this faster approach is as accurate as the other one. This will be done in the next sections.

5.2.4 Analysis of the spatial convergence

To verify the order of the spatial convergence on a problem with an analytical solution, the three-dimensional cylindrical Couette flow is simulated (see Fig. 5.2). In this case, the fluid is Newtonian and only the inner cylinder is rotating. In the laminar regime, the stationary analytical solutions for the velocity, the norm of the shear rate and the power P are expressed as

$$u_\theta(r) = \omega \frac{(r_{in}r_{out})^2}{(r_{out}^2 - r_{in}^2)} \left(\frac{1}{r} - \frac{r}{r_{out}^2}\right) \tag{5.14}$$

$$\|\dot{\gamma}\| = 2\sqrt{2}\omega \frac{(r_{in}r_{out})^2}{(r_{out}^2 - r_{in}^2)} \frac{1}{r^2} \tag{5.15}$$

$$P = 4\pi\mu\omega^2 \frac{(r_{in}r_{out})^2}{(r_{out}^2 - r_{in}^2)} h \tag{5.16}$$

where r is the radial position, r_{in} and r_{out} are the radii of the inner and outer cylinders, and h is the height of the fluid.
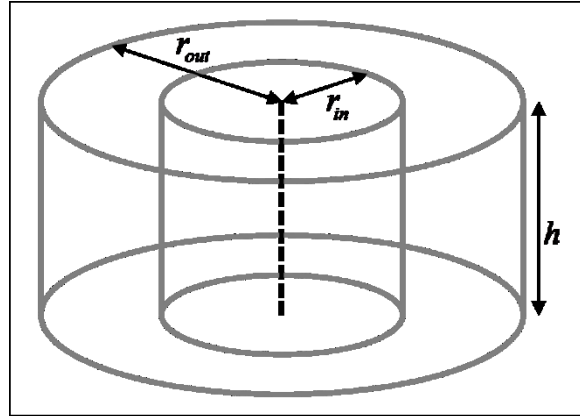
Figure 5.2: Geometry of the Couette flow problem.

The Reynolds number is set to one and the emphasis is put on the impact of the lattice spacing on the accuracy of the scheme. The boundary conditions for the inner and outer cylinders are defined by the extrapolation method. As presented in Section 5.2.3.2, the two different approaches to compute the power (using the shear rate or the torque) are compared. The deviation from the analytical solution is computed as $e = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\frac{(\alpha-\alpha^*)^2}{(\alpha^*)^2}}$, where n stands for the total number of

fluid lattice nodes and the symbol "*" denotes the analytical solution of the quantity α under investigation.

5.2.4.1 Circular Couette flow with periodic boundary conditions

In this case, the boundary conditions for the top and bottom are set as periodic. The velocities of the inner and outer cylinders are imposed by means of the extrapolation method. The accuracy of the LBM scheme is determined for the velocity, shear rate and power. The errors on the velocity and norm of the shear rate are presented in Fig. 5.3(a), so that the order of the spatial convergence can be quantified as the slope of the straight line. This figure indicates that the scheme achieves second-order accuracy for the velocity (slope of 2.11), thereby verifying the adequacy of the implementation, as already discussed in our previous paper [140]. It also appears that the scheme is second order for the norm of the shear rate (slope of 1.84); these findings support what has already been shown in the literature [62]. In the same manner, the accuracy of the LBM scheme on the power is presented in Fig. 5.3(b). For the power computed from the torque, the scheme achieves second-order accuracy (slope of 2.07). Conversely, when the power is computed from the shear rate, the error does not monotonically decrease with the lattice spacing. Indeed, here the error on the power is dominated by the error on the volume of the fluid zone. More precisely, due to the use of a Cartesian structured mesh, the error on this volume is globally convergent but can vary locally (not shown here). Given that the power computed from the shear rate is based on a volume integral (see Eq. (5.10)), the error on the power can likewise be locally affected, notwithstanding the global convergence. From the results shown in Fig. 5.3(b), it seems that computing the power through the surface integral in Eq. (5.12) does not lead to local oscillations in the corresponding convergence curve.
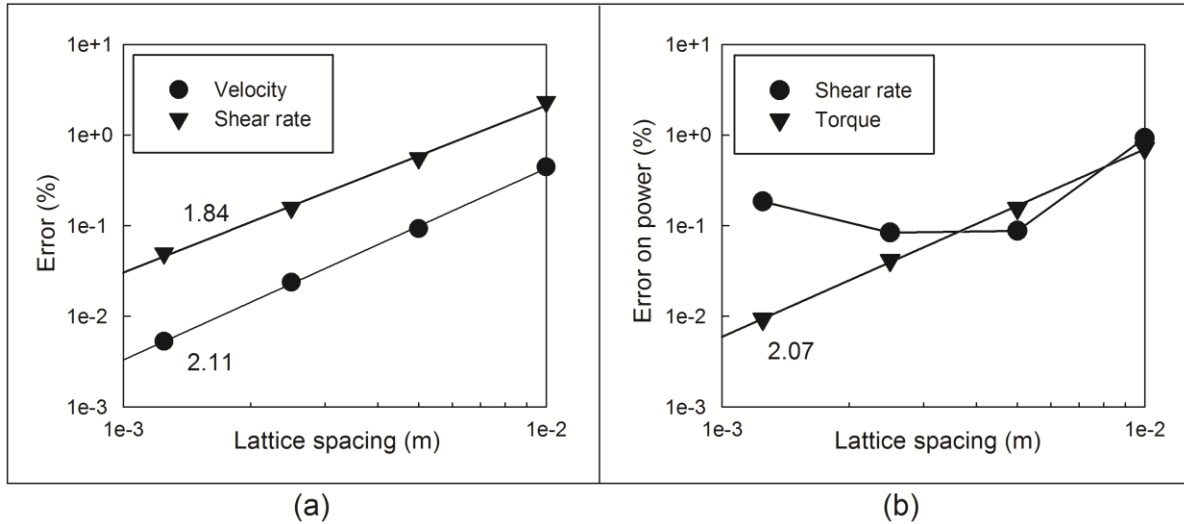
Figure 5.3: Convergence curves for the Couette problem with periodic boundary conditions: (a) velocity and shear rate, (b) power consumption from shear rate and torque values. The numbers correspond to the slopes of the straight lines.

5.2.4.2 Circular Couette flow with mixed boundary conditions

Here the boundary conditions at the top and bottom are modified to better approximate real mixing systems. To do so, free slip boundary conditions (i.e. u_r and u_θ are free and $u_z = 0$) are imposed at the top, mimicking a free surface. In addition, the analytical velocity defined by Eq. (5.14) is applied at the bottom with the extrapolation method. By means of such modifications (referred to as mixed boundary conditions), the impacts of the boundary conditions can be studied without modifying the stationary solution of the flow.

The errors on the velocity and norm of the shear rate are presented in Fig. 5.4(a). It appears that the scheme still achieves second-order accuracy for the velocity (slope of 2.13), thereby indicating that the modification of the boundary conditions does not globally modify the convergence of the computed velocity field. Conversely, the order of convergence is reduced to one for the norm of the shear rate (slope of 1.11), as opposed to two when periodic boundary conditions are used (Section 5.2.4.1). Fig. 5.4(b) shows that, once again, when the power is computed from the shear rate, it doesn't seem to be convergent (at least for $\delta x > 10^{-3}$). In addition, Fig. 5.4(b) also shows that the convergence is likewise reduced to the first order for the power computed from the torque (slope of 1.13), as opposed to two when periodic boundary conditions are used (Section 5.2.4.1). A similar reduction to the first order of accuracy for the

total force was also observed by Caiazzo et al. [146]. We believe these reductions on the convergence can be explained by local perturbations on the solution generated by the boundary conditions. For instance, an axial component of the velocity is created at the intersection between the cylinders and the bottom of the Couette geometry, where the extrapolation method is ill-defined (i.e. no second fluid lattice, see Section 5.2.3.1). Fig. 5.4(c) presents the values of the sum over the lattice nodes of the axial component of the velocity, denoted V_z^{tot}, versus the lattice spacing. Contrary to the periodic case, a small axial flow is indeed created, but fortunately, its value reduces as the square of the lattice spacing.
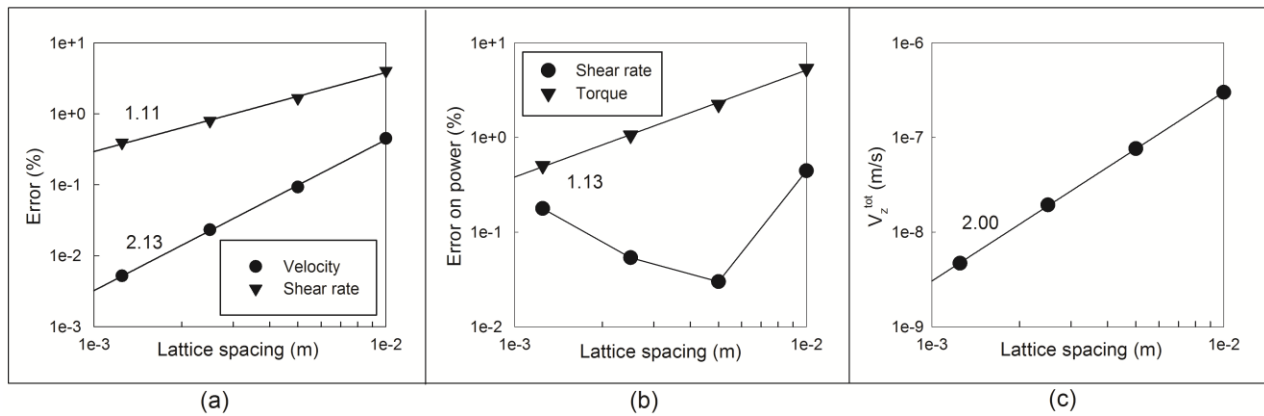
Figure 5.4: Convergence curves for the Couette flow problem with mixed boundary conditions: (a) velocity and shear rate, (b) power consumption and (c) sum over the lattice nodes of the axial component of the velocity, V_z^{tot}. The numbers correspond to the slopes of the straight lines.

In summary, we observe that a modification on boundary conditions can reduce the accuracy of the shear rate and the power, even if the scheme still achieves second-order accuracy for the velocity. These developments are important for simulations in more complex geometries, in that they suggest the convergence of the shear rate and the power will in all likelihood be reduced to first-order accuracy. Moreover, the power computation based on the torque (i.e. on the force) is seemingly more adequate owing to its monotonically decreasing convergence behavior. A similar conclusion was drawn by Mei et al. [89] for the computation of drag coefficients over cylinders and spheres, where the computation based on the force was found to be more accurate than the stress integration over the surface of the obstacle. Finally, it appears that a numerical axial flow can be generated by local perturbations on the velocity field, when the extrapolation method is ill-defined. This result must be kept in mind as the axial flow is used to characterize the pumping capacity of a mixing system.

5.2.5 Simulation results for the Maxblend mixer

A parallel implementation of the LBM presented in Section 5.2.3 was used to simulate fluid flow within a Maxblend mixing system. First, for the unbaffled configuration, the accuracy of the simulation process is characterized, as well as the impacts of the bottom clearance on the pumping capacity and power consumption. Following these results, the analysis is extended to determine the optimum values of the bottom clearance for different Reynolds numbers. Next, the accuracy of the power consumption is investigated in the case of the baffled configuration. This case is more complex in terms of the geometry and simulation process, in that it requires simulating the motion of the impeller with respect to the baffles.

5.2.5.1 Methodology

The Maxblend mixer considered in this work is the wedge impeller configuration, as presented in Fig. 5.5(a). It can be used with or without baffles, depending on the flow regime. The geometrical characteristics of the mixing system and the physical properties of the fluid are provided in Table 5.2. As an illustration, the velocity profile at $Re = 120$ in the unbaffled configuration is given in Fig. 5.5(b).

(a)   (b)
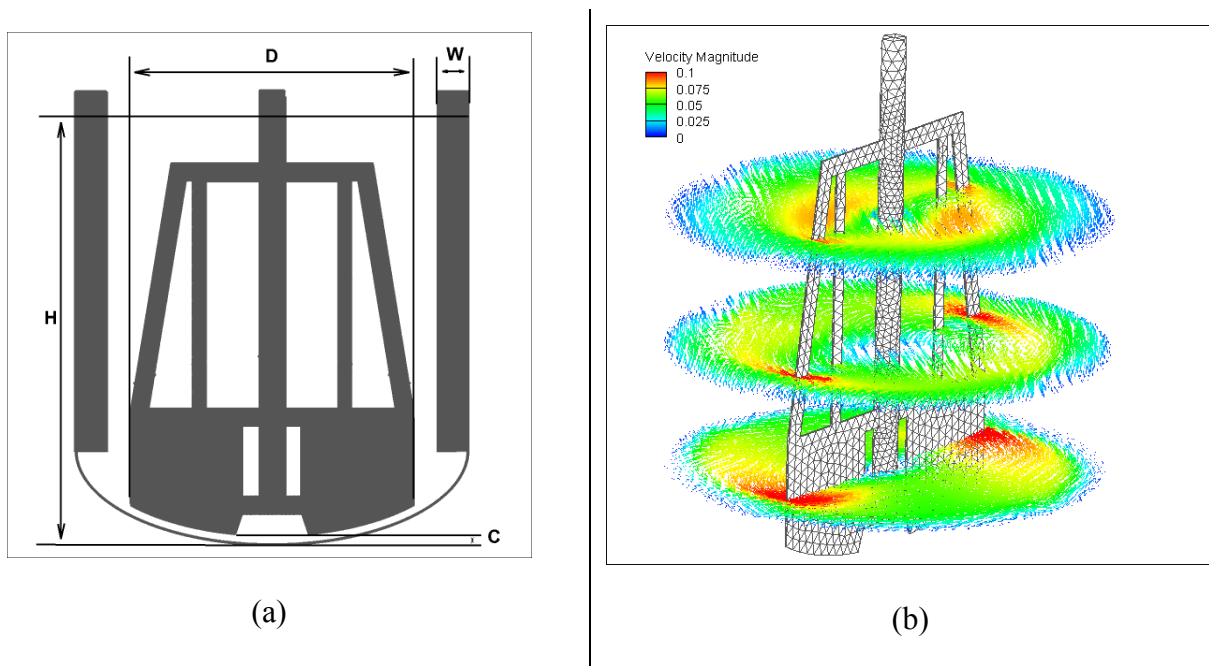
Figure 5.5 : The Maxblend impeller (wedge configuration): (a) geometry and (b) illustration of the velocity profile at Re=120.

In the case of a mixing system, the Reynolds number is defined as $Re = \rho N D^2/\mu$, where N is the rotational speed (in RPS) and D is the impeller diameter. The variation of the Reynolds number is achieved by adjusting the rotational speed. For impeller comparison purposes [35, 36, 143], the power consumption P is generally represented by the dimensionless power number N_p, defined as $N_p = P/\rho N^3 D^5$. As it is constant is the turbulent regime, it can be used to compare the efficiency of mixing systems designed for low viscosity fluids. Conversely, the power constant $K_p = P/\mu N^2 D^3 = N_p.Re$, is constant in the laminar regime. It can then be used for the comparison of mixing systems designed for high viscosity fluids.

Tableau 5.2: Geometrical characteristics of the Maxblend mixing system and physical properties of the fluid.

c_0	Standard bottom clearance	5.5 mm
D	Impeller diameter	255 mm
H	Fluid height	410 mm
W	Baffle width	26 mm
T	Tank diameter	356 mm
V	Vessel capacity	35.4 L
ρ	Fluid density	1240 kg. m^{-3}
μ	Fluid viscosity	0.1 Pa.s

The pumping capacity of the mixing system is also represented by a dimensionless number, the axial flow number $N_q = Q_z^+/ND^3$, where the axial pumping Q_z^+ is given by

$$Q_z^+ = \frac{1}{H}\int_V u_z^+ dv \tag{5.17}$$

In this expression, H is the fluid height, V is the total fluid volume and u_z^+ is the upward axial component of the velocity [13].

In this work, two types of simulation strategies were used depending on the topology of the flow domain. To begin with, if the topology is fixed (i.e. the shape of the fluid domain is fixed in time), the simulation process can be simplified by the use of a Lagrangian frame of reference. For instance, the simulation of the unbaffled mixing system can be done with a frame of reference attached to the impeller. Owing to this change of frame, there is no need to simulate the motion of the impeller and the discretization process (selection of solid and fluid lattice nodes) is done only once. Because such a frame of reference is in acceleration, a body force $\vec{g}(\vec{x}, t)$ is used to add the Coriolis and centrifugal forces:

$$\vec{g}(\vec{x}, t) = -2\vec{\omega} \times \vec{u}(\vec{x}, t) - \vec{\omega} \times \vec{\omega} \times \vec{r} \tag{5.18}$$

where $\vec{\omega}$ is the rotational velocity vector (in $rad.s^{-1}$) and $\vec{r}$ is the radius. However, if the topology of the flow domain is time dependent, as with the baffled configuration, the Lagrangian frame of reference can no longer be used. The simulation strategy is then complexified by the need to simulate the motion of the impeller. This modification implies re-doing the discretization process (i.e. selection of fluid and solid lattice nodes) at each time step and initializing the new fluid lattice nodes. To do so, we have chosen to use the so called non-equilibrium corrected refill [88] in order to minimize oscillations around the impeller. We will come back to this point in Section 5.2.5.3.

As mentioned in Section 5.2.3.1, all the boundary conditions, except those at the free surface, are imposed with the extrapolation method. This boundary condition strategy requires computing the fractions Δ during the discretization process. The fractions used to describe the tank walls are computed analytically, while a surface mesh is used to compute the fractions for the impeller. At the top of the tank, the free surface of the fluid is modeled by a free slip boundary condition (i.e. u_r and u_θ are free and $u_z = 0$). This approximation has been commonly used in laminar and transitional regimes when the Froude number $F_r = N^2 D/g$ is small.

The simulations were performed on Calcul Quebec Colosse and Mammouth-Parallèle II supercomputers, the characteristics of which are summarized in Table 5.3.

Tableau 5.3: Characteristics of the supercomputers used for the simulations.

Characteristics	Colosse supercomputer	Mammouth-Parallèle II
Number of nodes	960	1588
Type of nodes	2 Intel Nehalem-Ep 4-core proc.	2 AMD Opteron 12-core proc.
Total number of cores	7680	38112
Memory per node	24 GB	32 GB
Total available memory	23 TB	50.8 TB
Network	Infiniband QDR (40 Gb/s)	Infiniband QDR (4 Gb/s)
Peak performance	88 Tflops	333 Tflops

5.2.5.2   Effect of bottom clearance

This section is primarily concerned with the suitability of the LBM to model a small variation of the bottom clearance. The Lagrangian frame of reference was used to simulate the stationary flow of the unbaffled mixing configuration. The simulation was stopped when the relative variation of the flow field was lower than 10^{-5}. The selected lattice spacing δx is equal to 1.25 mm (yielding more than 19 million fluid lattice nodes), as preliminary results showed that, compared to finer lattice spacings, the variations on the power constant and axial flow number were lower than 2% and 1%, respectively. The three selected values of the Reynolds number (7, 33 and 68) are representative of typical conditions of viscous mixing in laminar and transitional regimes. The relaxation parameter τ of the lattice Boltzmann equation (see Eq. (5.6)), was adjusted to ensure low Mach numbers, thereby limiting compressibility errors. However, this selection leads to a compromise between accuracy and computational time, as the simulation time drastically increases when $\tau \rightarrow 0.5$. Thus, the maximum Mach numbers were 3.10^{-2} for $Re = 7$ and 6.10^{-2} for the two larger Reynolds numbers (33 and 68), which are small enough to ensure good accuracy (see Section 5.2.3). The computations were performed on Colosse supercomputer for an average computational time of 7 hours with 64 cores.

5.2.5.2.1   Standard bottom clearance

First, it is essential to ensure the accuracy of the simulation strategy. To accomplish this, our results are compared with experimental data from Fradette et al. [143] and simulation results obtained with the finite element method (FEM) by Devals et al. [13]. The values of the corresponding power constant for the standard bottom clearance ($c_0 = 5.5\ mm$), referred to as $K_p^0 = K_p(c_0)$, are summarized in Table 5.4. Surprisingly enough, with the LBM, the power constants computed from the shear rate ($K_p^0 = 158$) and torque ($K_p^0 = 160$) are quite similar. The difference is rather small considering that the computation based on the shear rate was shown to be not monotonically convergent in Section 5.2.4. These results exhibit a good agreement with the experimental data ($K_p^0 = 164$), corresponding to a maximum difference of 4%, which is within the experimental error (of the order of $\pm10\%$). On the other hand, with the FEM ($K_p^0 = 177$), the difference is more significant (+8%), but can be explained by differences in design parameters. For instance, the ratio between the diameters of the tank and impeller is 5% lower in the FEM simulations.

Tableau 5.4: Values of the power constant for the standard bottom clearance obtained with the LBM, with the FEM [13] and measured experimentally [143].

Method	LBM	FEM	Experimental data
K_p^0	158 from shear rate (-4%) 160 from torque (-2%)	177 (+8%)	164

5.2.5.2.2   Impact of the bottom clearance

Knowing the accuracy of the LBM on K_p^0, we can now focus on the impact of the bottom clearance on the power consumption. Fig. 5.6(a) shows the variation of the normalized power constant $K_p(c)/K_p^0$ versus the normalized bottom clearance c/c_0, for results obtained with the LBM and the FEM as well as experimental data. Notice that the curves computed from the torque and the shear rate are almost identical. Furthermore, a good agreement is observed between the LBM and FEM results, since the sole significant differences are obtained for the smallest bottom

clearance, where numerical errors are higher (fewer elements between the impeller and the tank wall). A rather good agreement is also observed with the experimental data. The differences can be explained by the experimental error on the bottom clearance ($\pm 1\ mm$, i.e. 20% of c_0). This rather large experimental error is due to the technical difficulty of accurately positioning the impeller, as it is directly attached to the motor.
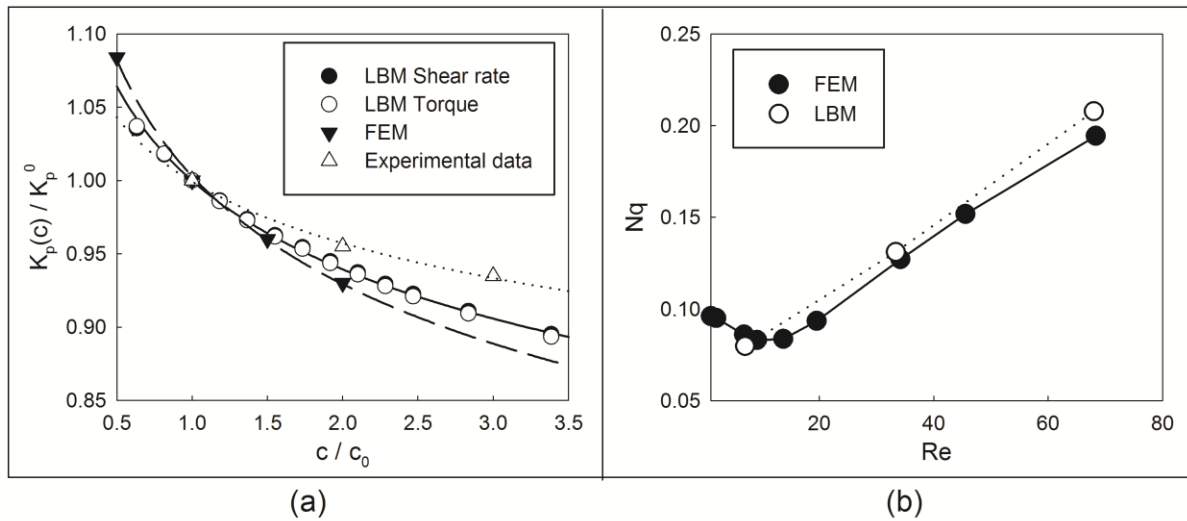
Figure 5.6: Comparison of LBM, FEM [13] and experimental data [143] for (a) the impact of the bottom clearance on the power constant and (b) the impact of the Reynolds number on the axial flow number.

It is also important to verify the accuracy of the LBM on the pumping capacity. This is crucial because it was shown in Section 5.2.4.2 that the boundary conditions used for the LBM can generate an erroneous numerical pumping. Fig. 5.6(b) displays the evolution of the axial flow number N_q versus Re for results obtained with the LBM and the FEM. A good agreement is observed, as the differences are equal to 7.9%, 2.9% and 6.5% for the Reynolds numbers of 7, 33 and 68, respectively. Moreover, it shows that the LBM and FEM exhibit the same linear behavior for $Re > 7$.

The results above show that the power consumption and pumping capacity simulated with the LBM, combined with the extrapolation method, are consistent with experimental data and FEM simulation results. Furthermore, the method used to compute the power (from the shear rate or the torque) does not significantly impact the accuracy of the power consumption itself or its dependency on the bottom clearance. Note that all power values reported in the remainder of this

paper were calculated form the torque. Finally, these results indicate that the erroneous pumping inherent to the boundary conditions and the extrapolation method, as discussed in Section 5.2.4.2, is small and does not significantly affect the pumping behavior predicted by the LBM.

5.2.5.2.3 Optimum bottom clearance

We showed in the previous section that the LBM can predict accurately the impact of a variation of the geometry on the power consumption and the pumping capacity. For the sake of completeness, the simulation work was extended to determine an optimum bottom clearance in regard to these two macroscopic quantities, and show by the same token that the LBM can be used for design and optimization purposes.

First, the impact of the bottom clearance on the power consumption is considered. Fig. 5.7(a) compares the variation of the normalized power number $N_p(c)/N_p^0$ versus c/c_0, for three Reynolds numbers (7, 33 and 68), where the power number at the standard bottom clearance is referred to as $N_p^0 = N_p(c_0)$. According to these curves, the impact on the power increases inversely with the bottom clearance. In addition, for normalized bottom clearance values lower than 1.5, the variation is independent of the Reynolds number. Conversely, for $c/c_0 > 1.5$, the impact on the power consumption is lower for the largest value of the Reynolds number ($Re = 68$). One possible explanation for the different behavior observed at $Re = 68$ is the likely increasing impact of inertia on the hydrodynamics when the clearance increases. In the same manner, Fig. 5.7(b) shows the variation of the normalized pumping number $N_q(c)/N_q^0$ with respect to the bottom clearance, where the axial flow number at the standard bottom clearance is referred to as $N_q^0 = N_q(c_0)$. It can be observed that the profile is quasi-linear and the impact of the bottom clearance is inversely proportional to the Reynolds number. Lastly, considering that the pumping plays an important role in the homogeneity of a mixture and that the power consumption represents its cost, it is worthwhile to investigate the ratio $\frac{N_q(c)}{N_p(c)}\frac{N_p^0}{N_q^0}$, as was done in the experimental work of Guntzburger et al. [35]. We believe that this ratio, which characterizes the efficiency of the mixing process, may be used to determine an optimum bottom clearance. From Fig. 5.7(c), it can be noticed that, in the laminar regime ($Re = 7$), the optimal value of the normalized bottom clearance is between 0.8 and 1.4, therefore confirming the standard bottom clearance ($c/c_0 = 1$) is a good choice. However, in the transitional regime ($Re = 33$ and 68), the

optimum value is situated between 1.4 and 2, which suggests that the standard bottom clearance is not adequately large enough. It is noteworthy that, compared to the laminar regime, the impact of the bottom clearance is globally reduced in the transitional regime. We believe these results are highly significant for the minimization of the power consumption, given that the standard bottom clearance is one of the most relevant design parameters of the Maxblend [143]. It also confirms that the LBM is useful to investigate small variations of design parameters.
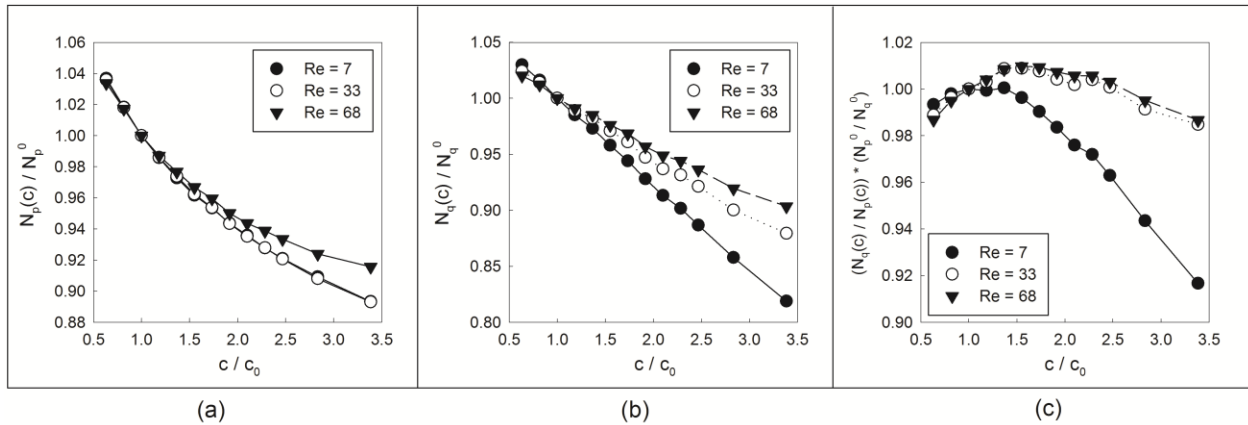
Figure 5.7: Impact of the bottom clearance on (a) the power number, (b) the axial flow number and (c) their ratio, for Reynolds numbers of 7, 33 and 68.

5.2.5.3 Simulation of rotating impeller

The objective is now to characterize the accuracy of the simulation process in the case of the baffled configuration. The emphasis is put on the impact of the lattice spacing on the power consumption and on the comparison of the two different approaches to compute the power (i.e. from the torque and shear rate). Since the Lagrangian frame of reference can no longer be used, the position of the solid part (i.e. the impeller) is not fixed in time. Therefore, the discretization process (i.e. selection of fluid and solid lattice nodes) must be applied at each time step, thereby possibly increasing significantly the total computational time. The motion of the solid part also requires initializing the new fluid nodes. Unfortunately, given their mesoscopic nature, there is no analytic definition of the populations f_k for a given velocity, hence no analytical initialization (or refill) exists. Given that simple refill methods using the equilibrium population [87] generally generate inaccuracies and oscillations around moving obstacles, we have chosen to use a more elaborate approach, the so-called non-equilibrium corrected refill [88]. More precisely, as in the case of the extrapolation method (see Section 5.2.3.1), it is based on the decomposition of the

populations into equilibrium and non-equilibrium parts to determine unknown populations. Similarly, the equilibrium part is computed by means of Eq. (5.5) with an extrapolated velocity. The non-equilibrium part is directly copied from that at a neighboring fluid node. In our case, the direction used to extrapolate the velocity and select the neighboring fluid node is that countercurrent to the flow. On account of this approach, oscillations around moving obstacles are minimized and the accuracy of the force computation is enhanced [88].

Three selected lattice spacings were considered: $\delta x_1 = 2.5\ mm$, $\delta x_2 = 1.77\ mm$ and $\delta x_3 = 1.25\ mm$. The Reynolds numbers are $Re = 7$ and 120, for which experimental data [143] and FEM results [13] are available. As mentioned in the previous section, the relaxation parameter τ was adjusted for the Mach number, resulting in a maximum Mach number lower than $7.5 * 10^{-2}$. The selected bottom clearance is $c = 2c_0$ in order to limit inaccuracies at the bottom of the mixing system. As the lattice spacings are small compared to the distance covered by the impeller during one time step δt, the discretization process (see Section 5.2.5.1) was only applied every 5 iterations in order to reduce the computational cost. Note that this choice was observed to yield adequate results. The total simulation time corresponds to 3 and 10 complete revolutions of the impeller for the Reynolds numbers of 7 and 120, respectively. All computations were performed on Mammouth-Parallèle II supercomputer. For the 3 impeller revolutions, the average computational time was 10 hours on 72 cores for δx_1, 16 hours on 96 cores for δx_2 and 28 hours on 120 cores for δx_3. These rather large computational times can be explained by the non-stationary nature of the solutions, which require re-doing the discretization process and computing the power regularly throughout the simulation. As mentioned earlier, these two procedures are time consuming and may constitute a significant portion of the total computational time (up to 60 % in our tests).

In order to determine the accuracy of the results, the unbaffled configuration was simulated at $Re = 7$. In this case, the stationary result obtained in the previous section (i.e. with the Lagrangian frame of reference) is considered to be the most accurate result and is referred to as N_p^{ref}. For instance, Fig. 5.8 denotes the evolution of the power number for the largest lattice spacing δx_1. Apparently, contrary to what was observed in Section 5.2.5.2, the method used to compute the power greatly impacts its variation in time, in that the power computed from the torque is largely more affected by oscillations. This difference can be explained by the fact that

the torque is computed as a surface integral of the force on the impeller (see Eq. (5.11)), where the refill of the new fluid nodes generates oscillations. Conversely, when the power is computed as a volume integral of the shear rate (see Eq. (5.10)), the number of lattice nodes affected by the refill is negligible compared to the total number of fluid nodes, thereby yielding a better accuracy.
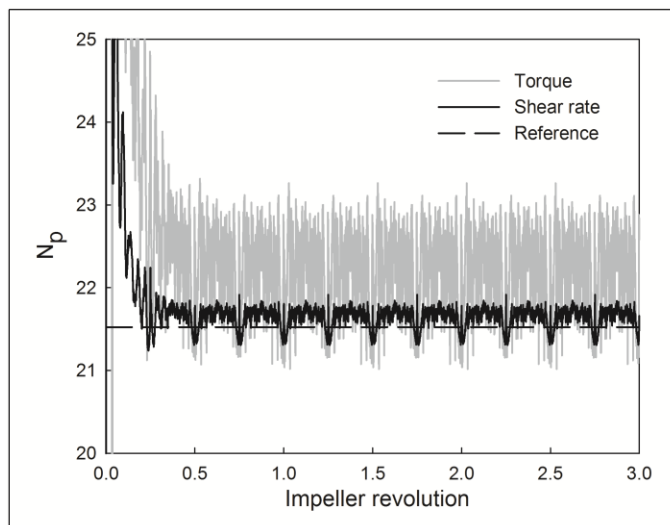
Figure 5.8: Evolution of the power number for the unbaffled configuration at Re=7 ($\delta x = 2.5\ mm$).

In order to investigate the impact of the lattice spacing, the variations of the average power number and the standard deviations of the power number are presented in Fig. 5.9. These data were computed over the last 2 revolutions when a quasi-steady state behavior was achieved. Fig. 5.9(a) shows that the results for the power number exhibit a good agreement with the reference solution $N_p^{ref} = 21.5$, with a maximum difference of 4.5%. More precisely, while the power is always overestimated by the two different approaches, the computation based on the shear rate yields the most accurate average value (maximum difference of 2.4%). In Fig 5.9(b), the standard deviation around the average power is 4 times higher with the torque computation, although it reduces for both approaches when the lattice spacing is reduced. To sum up, in the case of a moving solid part, the power computation based on the shear rate is seemingly more effective in that the average power value is more accurate and the oscillations are reduced. It is also important to underline that these oscillations are solely due to the initialization process of the new fluid nodes, considering that they did not appear when the Lagrangian frame of reference was used.
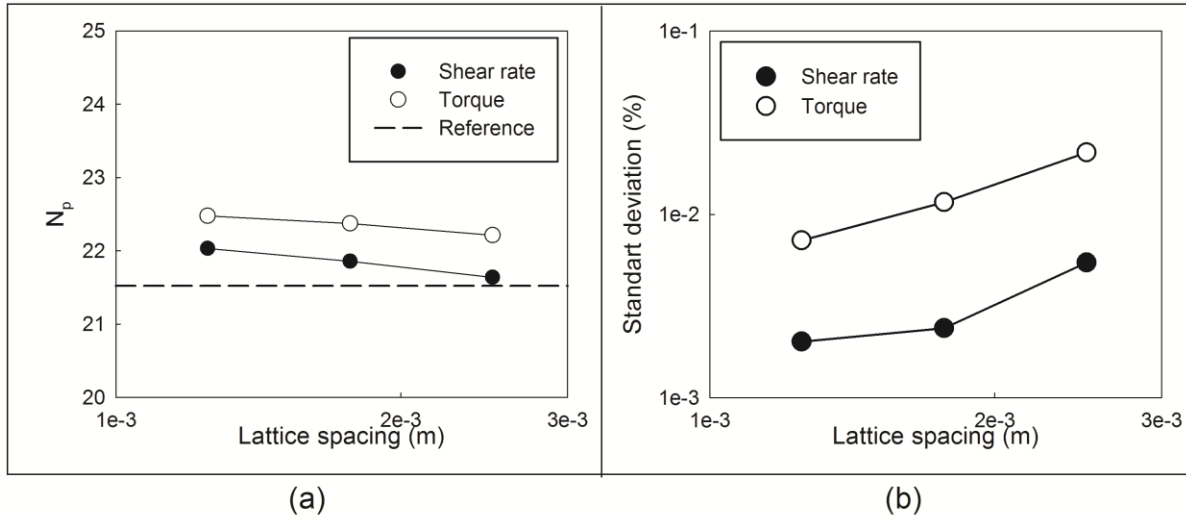
Figure 5.9: Variations with respect to the lattice spacing of (a) the average power number and (b) the standard deviation of the power number, for the unbaffled configuration at Re=7.

The results for the baffled and unbaffled configurations and a Reynolds number of 120 are next compared. Fig. 5.10 shows the evolution of the power during the last two revolutions for the largest lattice spacing δx_1. First, Fig. 5.10(a) presents the results for the unbaffled configuration. It can be noticed that, similarly to the results obtained at $Re = 7$ (Fig. 5.8), the power computed from the torque is largely more affected by oscillations. In addition, Fig. 5.10(b) shows that, for the baffled configuration, the evolution of the power is periodic with respect to the relative position of the impeller versus the baffles. A comparable evolution was observed with FEM results by Devals et al. [13], therefore they will be used to assess our LBM results. To this end, two mixing system parameters are considered: the increase in power consumption due to the baffles and the maximum variation of power during one impeller revolution.

Fig. 5.11(a) compares the increase in power obtained with the LBM (this work) and the FEM [13], as well as experimental data [143]. A good agreement is observed between the numerical results, as the LBM yields to an increase between 11.8 and 13.1%, and the FEM gives +12%. However, compared to experimental data (+8.5%), the impact of the baffles appears to be overestimated. In addition, Fig. 5.11(b) compares the maximum power amplitude by the LBM and FEM. Here, the power amplitude refers to the maximum amplitude of the power due to the motion of the impeller with respect to the baffles. In order to vanish the oscillations related to the refill procedure within the LBM, the variation of the power was smoothed with a moving average

over 20 iterations. According to these curves, it appears that only the amplitude obtained with the power computed from the shear rate (6%) is comparable to the FEM result (4%). Indeed, the amplitude is largely overestimated when the power is computed from the torque (>17.5%).

(a)

(b)
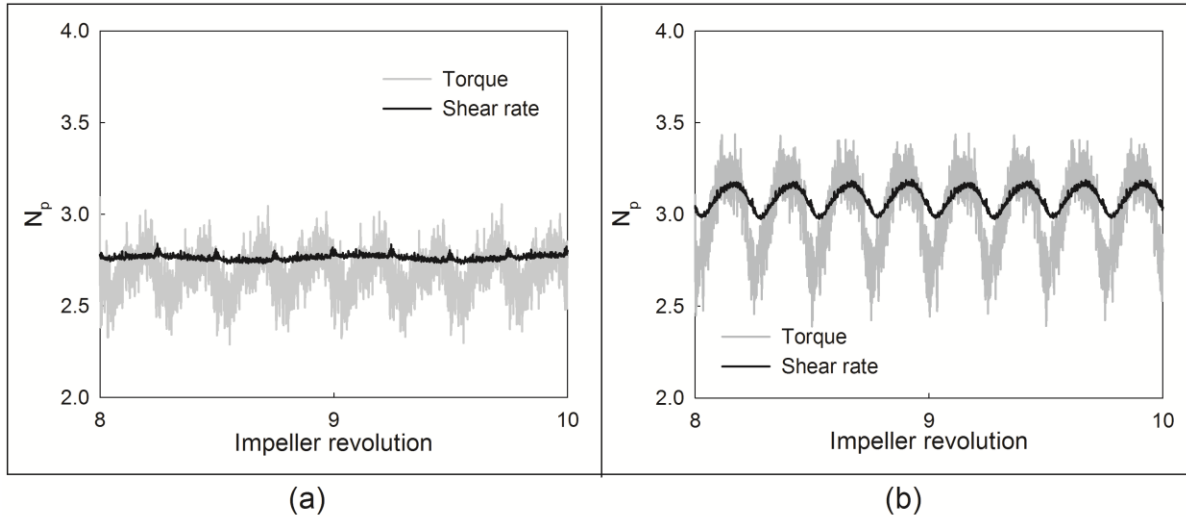
Figure 5.10: Evolution of the power number at Re=120 for (a) the unbaffled and (b) baffled configurations, with $\delta x = 2.5\ mm$.

(a)

(b)
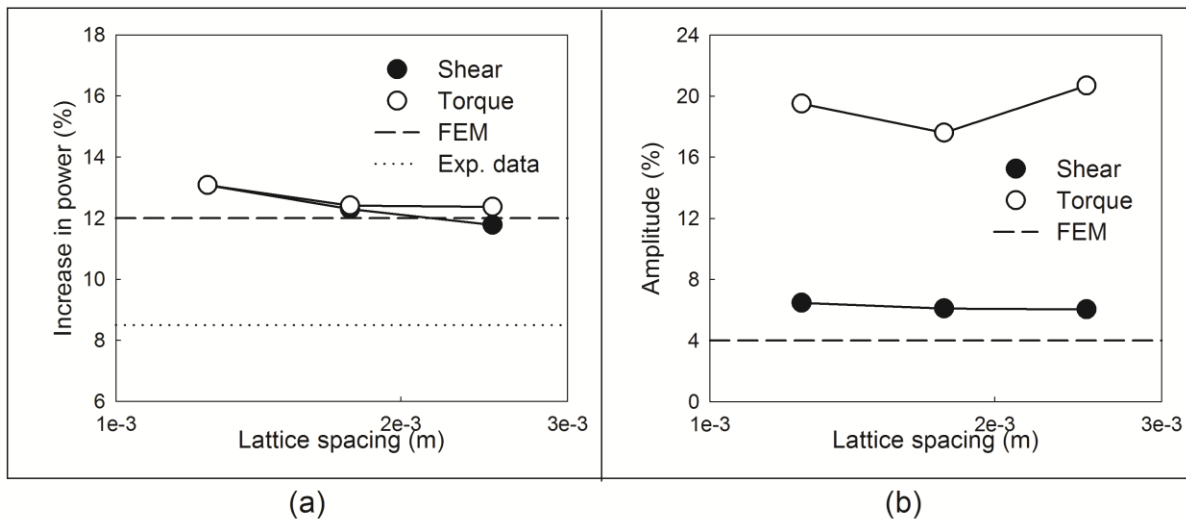
Figure 5.11: Variation of the power for the baffled configurations: (a) increase compared to the unbaffled configuration and (b) maximum amplitude during one revolution.

In summary, contrary to simulations for a fixed geometry (see Section 5.2.5.3), the selection of the method to compute the power can significantly impact the accuracy of the results around moving solid parts. When computed from the torque, the evolution of the power in time is largely

perturbed by oscillations. We believe these inaccuracies are due to the initialization procedure that is necessary when new fluid nodes appear. Conversely, when the power is computed from the shear rate, the LBM results agree well with the experimental data and the FEM results. For instance, the increase in power due to the baffles and the maximum amplitude that occurs during one impeller revolution are accurately simulated.

5.2.6 Concluding remarks

The objective of this work was to assess the suitability of the extrapolation method for the LBM simulation of viscous mixing flows involving complex geometries. To our knowledge, it is the first time that such extended accuracy analysis is presented for such complex 3D flow problems. The emphasis was put on the capacity to simulate accurate power consumption and pumping capacity for both unbaffled and baffled configurations of the Maxblend mixing system.

Thanks to the simulation of the Couette flow problem, the impact of the boundary conditions at the top and bottom was analyzed. The LBM scheme was observed to achieve second-order accuracy for the velocity, but the norm of the shear rate and power were found to be more sensitive to a change of boundary conditions. In fact, these inaccuracies were related to local perturbations appearing when boundary conditions are ill-defined. These results also showed that the power computed from the torque, contrary to that obtained from the shear rate, presents a monotonically decreasing convergence behavior.

A highly parallel LBM scheme was next used to simulate fluid flow within the Maxblend mixing system using a Lagrangian frame of reference. A good agreement with experimental data and finite element simulation results was found for the power consumption and the pumping capacity. Note that, in this case, the method used to compute the power (from the shear rate or the torque) does not significantly impact the accuracy of the power consumption. The analysis was then extended to determine the optimum bottom clearance for three different Reynolds numbers. The results suggest that the standard bottom clearance is well suited for the laminar regime, but a larger value would be more efficient for the transitional regime. Moreover, they confirm that the LBM is an adequate tool for the optimization of design parameters.

Lastly, the results obtained for the more geometrically complex case (baffled configuration) showed that the evolution in time of the power consumption can be affected by numerical

oscillations. These inaccuracies are related to the initialization procedure required for the treatment of the new fluid nodes that appear around the moving impeller. The power computed from the torque is more sensitive to these oscillations but, fortunately, their amplitude decreases when the lattice spacing is reduced.

5.2.7 Acknowledgments

5.3 Résultats complémentaires

Les résultats présentés dans cette section ont pour but de compléter l'étude de convergence spatiale sur le problème du Couette cylindrique, proposée dans la section 5.2.4. Plus précisément, nous allons nous intéresser à l'impact du facteur de relaxation τ sur la précision. Dans le cas des régimes transitoire ou turbulent, la valeur du facteur de relaxation doit être proche de 0.5 afin de conserver un nombre de Mach en dessous de 0.2, c'est-à-dire d'assurer la stabilité numérique et la précision du schéma LBM. Dans le cas des écoulements en régime laminaire, les nombres de Mach correspondants étant plus faibles, il y a plus de liberté sur la sélection de la valeur de τ.

Nous allons nous intéresser plus particulièrement au cas de l'écoulement de Couette cylindrique avec des conditions aux limites périodiques sur la hauteur (voir section 5.2.4.1), pour un nombre de Reynolds de 1. Ainsi, la figure 5.12 présente les erreurs sur la vitesse et sur le taux de cisaillement pour des facteurs de relaxation compris entre 0.6 et 1.4, les différentes courbes représentant les erreurs associées aux quatre tailles de lattice utilisées. Il ressort des figures 5.12(a), pour la vitesse, et 5.12(b), pour le taux de cisaillement, que les tendances sont similaires c'est-à-dire que l'erreur diminue en fonction de la taille de lattice (ordre 2, voir section 5.2.4.1) et que la valeur de τ optimale semble être située autour de 0.8 (entre 0.7 et 0.9). Avec un seul cas test, il n'est pas possible de déterminer si la valeur optimale de 0.8 est générique ou si elle dépend de la géométrie et des propriétés du fluide. Cependant, une valeur similaire ($\tau = 0.809$) a aussi été proposée par Zhao [147]. Basée sur une étude mathématique de LBGK et vérifiée sur

plusieurs cas tests, cette étude montre que cette valeur est un bon compromis entre la précision (sur la vitesse) et la stabilité, sans être toujours optimale.
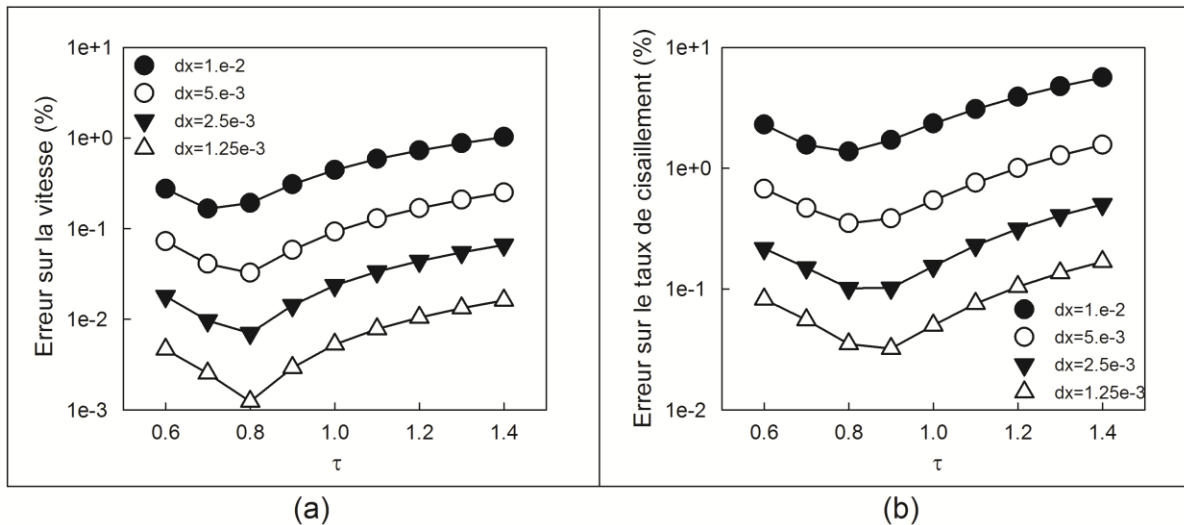
Figure 5.12 : Impact du facteur de relaxation τ sur la précision de (a) la vitesse et (b) du taux de cisaillement pour le problème de Couette.

Puisque le facteur de relaxation semble affecter la précision sur la vitesse et sur le taux de cisaillement de la même manière, il est intéressant d'étudier son impact sur d'autres grandeurs. Ainsi, la figure 5.13 présente les erreurs sur la puissance, calculée à partir (a) du taux de cisaillement et (b) du couple (voir section 5.2.3.2), pour des facteurs de relaxation compris entre 0.6 et 1.4. De la même manière, les différentes courbes représentent les erreurs associées aux quatre tailles de lattice utilisées. Pour la puissance calculée à partir du couple (figure 5.13(b)), on observe un comportement similaire à celui observé pour la vitesse et le taux de cisaillement, avec une valeur optimale de τ proche de 0.8. Dans le cas de la puissance calculée à partir du taux de cisaillement (figure 5.13(a)), le comportement est complètement différent. En effet, comme mentionné dans la section 5.2.4.1, l'erreur sur la puissance ne diminue pas avec la taille de lattice. On remarque même que pour la plus petite taille de lattice (dx=1.25e-3), la valeur de l'erreur n'est plus affectée par le facteur de relaxation. Cela confirme que, avec cette façon de calculer la puissance, l'erreur est dominée par un autre aspect.
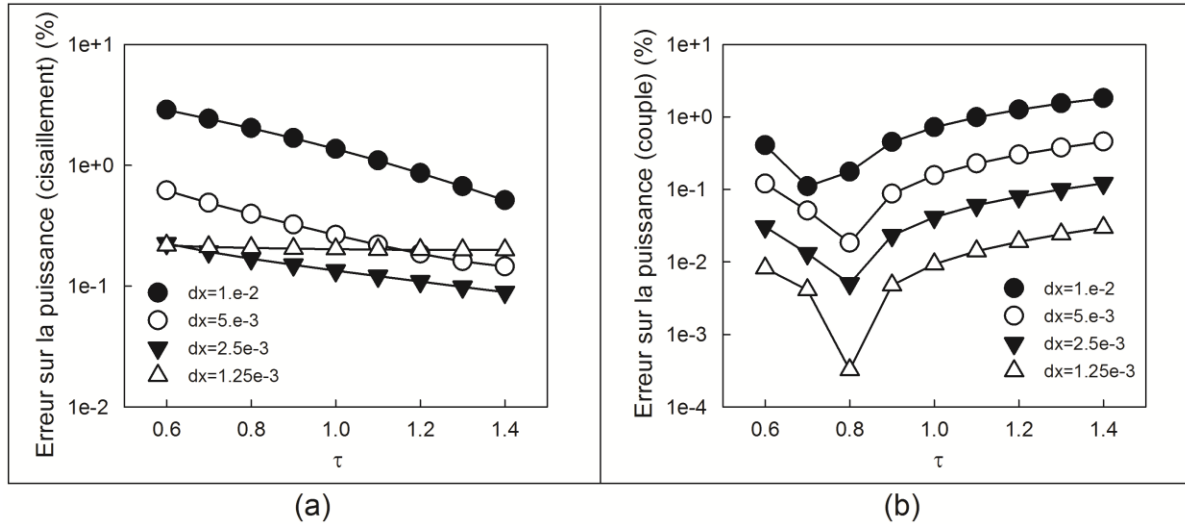
Figure 5.13: Impact du facteur de relaxation τ sur la précision de la puissance calculée à partir (a) du taux de cisaillement et (b) du couple pour le problème de Couette.

Comme nous l'avons mentionné dans la section 5.2.4.1, il semble que dans ce cas, le terme dominant soit l'erreur associé à l'intégration du volume. Afin de mieux comprendre cet aspect, la figure 5.14 présente l'erreur sur le volume en fonction de la taille de lattice. Il ressort que si le calcul du volume est globalement convergent, avec un ordre de précision proche de 2 (1.6), l'erreur ne diminue pas d'une façon monotone. Autrement dit, il n'est pas garanti que l'erreur sur le volume diminue pour une petite réduction de la taille de lattice, même si le volume est globalement convergent.

En conclusion, les résultats présentés dans cette section montrent qu'il existe une valeur du facteur de relaxation optimale (proche de 0.8), qui permet de minimiser l'erreur sur la vitesse, le taux de cisaillement et la puissance calculée à partir du couple. Dans le cas de la puissance calculée à partir du taux de cisaillement, l'erreur semble être dominée par l'erreur sur le volume. Plus précisément, comme l'erreur sur le volume ne diminue pas d'une façon monotone, la convergence spatiale de la puissance est largement perturbée.
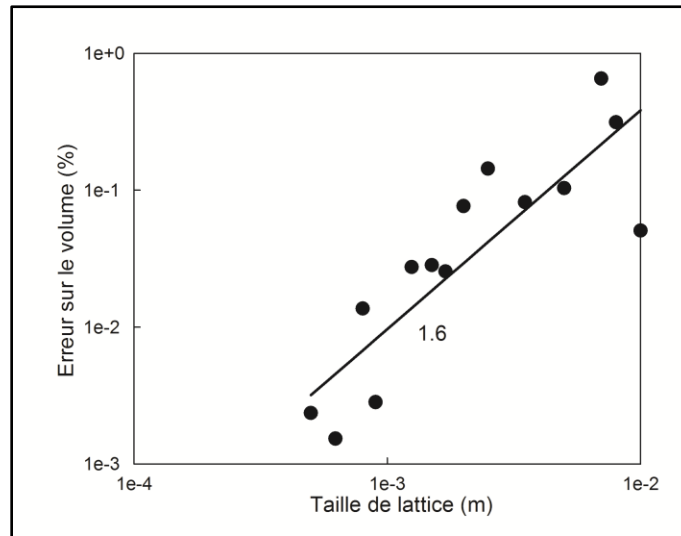
Figure 5.14: Erreur sur le volume en fonction de la taille de lattice pour le problème de Couette cylindrique.

CHAPITRE 6   APPLICABILITÉ DE LA LBM POUR LES RHÉOLOGIES COMPLEXES

6.1   Présentation du troisième article

Soumis à *The Canadian Journal of Chemical Engineering* le 8 Janvier 2013.

Auteurs : Vincent Stobiac, Louis Fradette, Philippe Tanguy, François Bertrand.

Cet article traite du mécanisme de pompage généré par le mélangeur Maxblend pour des liquides newtoniens et fortement rhéofluidifiants, ces derniers étant modélisés par le modèle de Carreau-Yasuda ($n = 0.05$). Plus précisément, les résultats présentés, obtenus avec la méthode de Boltzmann sur réseau (LBM), permettent de caractériser la forme de l'écoulement dans le régime laminaire profond. Ils permettent aussi d'apporter des éclaircissements sur des résultats expérimentaux récents, basés sur les méthodes de décoloration et de vélocimétrie par imagerie de particules (PIV). Tout d'abord, la variation du pompage dans le cas newtonien est étudiée et permet de souligner les limitations de la PIV bidimensionnelle. Cette étude montre que la variation du pompage est reliée à un changement dans la structure de l'écoulement secondaire (composantes axiales et radiales de l'écoulement). Ensuite, l'étude sur le pompage est étendue aux fluides fortement non newtoniens. Il ressort que le changement dans la structure de l'écoulement secondaire, observé dans le cas newtonien, est aussi présent et qu'il entraine la création de zones avec des fortes disparités de viscosité apparente. La forme de ces zones permet d'expliquer les patrons d'écoulements problématiques observés expérimentalement.

6.2 Pumping characterization of the Maxblend impeller for Newtonian and strongly non-Newtonian fluids

6.2.1 Summary

This paper examines the pumping mechanism generated by the Maxblend impeller for Newtonian and strongly shear-thinning fluids, the latter based on the Carreau-Yasuda model ($n = 0.05$). More precisely, results obtained with the lattice Boltzmann method (LBM) are presented and used to characterize the flow in the deep laminar regime. These LBM results revisit and contribute to understanding recent experimental data from the decolorization method and particle image velocimetry (PIV). First, the modification of the pumping of the Newtonian fluid in the deep laminar regime is assessed and the limitations of the two-dimensional PIV are discussed. This work clearly shows that the variation of the pumping is related to a change in the structure of the secondary radial and axial flow. Second, the analysis of the pumping is extended to highly non-Newtonian fluids and a similar transition is observed in the laminar regime. This phenomenon leads to the creation of zones with very different apparent viscosities, thereby explaining problematic flow patterns observed experimentally.

6.2.2 Introduction

Among the various impellers used in chemical industries, the Maxblend mixer (Sumitomo Heavy Industries, Japan) is an interesting candidate for mixing processes involving a wide range of viscosities. Despite a rather simple geometry, comprised of a lower large paddle and an upper grid, good performance has been observed from the laminar to the turbulent regimes. When compared to the helical ribbon and anchor at low Reynolds number [43, 148, 149] or to turbines in the turbulent regime [35, 148-152], the Maxblend provides a good compromise between mixing efficiency and power consumption. It has been successfully applied to many applications such as polymerization [152], bacterial culture [148, 150], gas dispersion [152] and solid suspension [151, 153].

Several experimental and numerical investigations on the Maxblend have been published regarding the impact of design parameters in terms of power consumption [13, 33, 36, 143], mixing time [33, 36, 143] and dispersive performance [43]. These studies have been carried out for both Newtonian and non-Newtonian fluids. Owing to such works, the performance of the

Maxblend is well documented, thus confirming the advantages and drawbacks of the impeller. In particular, if it has been established that the homogeneity of the mixture is harder to obtain at low Reynolds number [13, 36, 143, 154], the understanding of the mixing mechanisms in the deep laminar regime being still limited.

As the pumping capacity is a key factor for the mixing uniformity, Computational Fluid Dynamics (CFD) has been used to characterize the performance of the Maxblend in terms of pumping for Newtonian and non-Newtonian fluids. For instance, results obtained with the Finite Element Method (FEM) showed that the axial flow is characterized by a downward flow around the Maxblend and an upward flow near the tank walls [13, 36]. Although the shape of the axial pumping volume is toroidal and rather independent of the flow regime, the pumping efficiency is however largely affected by the Reynolds number [13, 43, 155], the rheology [13] and the bottom clearance [13, 155]. In addition, Devals et al. [13] noticed that the pumping is reduced at low Reynolds number and this effect seems to be amplified by the rheology. Nevertheless, they did not give any reason for this reduction.

From an experimental standpoint, the determination of the pumping capacity is complex due to the difficulty in measuring the flow field. However, two promising approaches, based on two-dimensional Particle Image Velocimetry (PIV) [156, 157] and the so-called decolorization method [32], have recently been utilized [35, 154]. With the 2D PIV, the flow is obtained through a statistical analysis of successive pictures representing the positions of particles in the system. On the other hand, the decolorization method measures the pumping indirectly. The idea is to extract the maximum pumping capacity from a decolorization curve, while taking into consideration that the decolorization rate is proportional to the pumping rate. The decolorization comes from the agitation of a small quantity of a neutrally buoyant acid solution to the liquid in the tank, which was initially rendered alkaline by the addition of a base. These recent experimental studies on the Maxblend are highly relevant given that they investigate the mixing of strongly non-Newtonian fluids, which are often encountered in industries (food, plastic and cell culture) yet rarely studied by researchers. The results confirm the toroidal shape of the axial pumping volume generated by the Maxblend impeller in the Newtonian case. They also highlight the occurrence of problematic flow patterns, which give rise to segregation zones indicative of inefficient mixing, for strongly shear-thinning fluids ($n = 0.05$) at low Reynolds number.

The Lattice Boltzmann Method (LBM) [58, 144] has been shown to be an adequate tool for the simulation of industrial mixing flows. In particular, this method was successfully used for the characterization of flow fields in Rushton turbine systems [27, 86], a crystallizer with a Rushton turbine [117], a standard anchor [140] and a Paravisc impeller [140]. Note that we recently investigated the accuracy of the LBM in the case of the Maxblend mixing system [155]. A thorough investigation of the simulation procedure was provided, thereby confirming the accuracy of the LBM predictions for Newtonian fluids.

From this literature review, it appears that, in the deep laminar regime, the understanding of the mechanisms inherent to the pumping generated by the Maxblend impeller is limited. The objective of this work is then to shed light on these mechanisms for Newtonian and strongly non-Newtonian fluids. To do so, LBM results are first validated with previously published FEM data [13]. These results are next used to revisit and better understand recent experimental data based on 2D PIV [154] and the decolorization method [35]. The limitations of these experimental approaches are highlighted and explained. To our knowledge, no such extended numerical investigation of the pumping capacity of the Maxblend has been done for Newtonian and strongly non-Newtonian fluids.

The paper is organized as follows: Section 6.2.3 details the geometry of the Maxblend impeller system as well as the rheology of the fluids used in this work. The LBM is also briefly presented along with a few comments regarding its implementation. In Section 6.2.4, results obtained with the LBM are compared to FEM numerical results and experimental data. In the case of the Newtonian fluid, the variation of the pumping with respect to the Reynolds number is studied by comparing velocity profiles. Finally, in the case of the strongly non-Newtonian fluids, a similar comparison is made and extended to the analysis of viscosity profiles.

6.2.3 Methodology

6.2.3.1 The Maxblend impeller

The mixing system used in this work is comprised of a wedged Maxblend impeller, a tank with an elliptical bottom and two baffles, as recommended by [33]. The geometry is presented in Fig. 6.1 and its characteristics are given in Table 6.1. The impeller is composed of a large paddle at the bottom, creating the pumping in the mixer, and an upper grid for dispersion purposes.
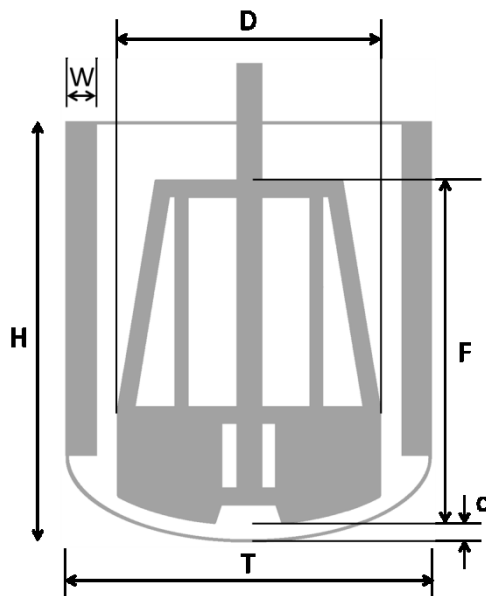
Figure 6.1: Geometry of the Maxblend mixing system.

Tableau 6.1: Geometrical characteristics of the Maxblend mixing system.

c	Bottom clearance	5.5 mm
D	Impeller diameter	255 mm
F	Impeller height	338 mm
H	Fluid height	410 mm
W	Baffle width	26 mm
T	Tank diameter	356 mm
V	Vessel capacity	35.4 L

6.2.3.2 Rheology of the fluids

Two different rheology models are considered in this work to simulate Newtonian and strongly non-Newtonian behaviors. The first one models a Newtonian diluted corn syrup, which is simply described by a constant viscosity. Following our recent experimental work [35, 154], the

Carreau-Yasuda model is used to describe the strongly non-Newtonian behavior of Steol solutions containing more than 2 wt% of NaCl. The Carreau-Yasuda model [11] is defined as

$$\eta(\dot\gamma) = \eta_\infty + (\eta_0 - \eta_\infty)[1 + (\lambda\dot\gamma)^a]^{\frac{n-1}{a}} \qquad (6.1)$$

where $\dot\gamma$ is the shear rate (in s^{-1}) defined by $\dot\gamma = \sqrt{2S{:}S}$, with $S = (\nabla\vec{u} + \nabla^T\vec{u})/2$ the shear rate tensor. The parameters of the model are η_0 and η_∞, the zero and the infinite shear rate viscosities (in $Pa.s$), respectively, λ the characteristic time of the fluid (in s), n the power law index and a characterizing the transition between the Newtonian and shear-thinning behavior.

Tableau 6.2: Values of the rheological parameters for the Newtonian and non-Newtonian fluids.

Fluid number	Rheological model	Density $(Kg.m^3)$	η_0 (Pa.s)	λ (s)	n (-)	a (-)	NaCl concentration (wt %)
1	Newtonian	1390	7.2	-	-	-	-
2	Newtonian	1370	1.3	-	-	-	-
3	Carreau-Yasuda	1030	7.1	0.053	0.05	2.2	2.1
4	Carreau-Yasuda	1030	17.8	0.17	0.05	5.3	2.7
5	Carreau-Yasuda	1030	46.5	0.63	0.05	10	2.5

As presented in Fig. 6.2, the fluid exhibits a highly shear-thinning behavior ($n = 0.05$) when $\dot\gamma$ exceeds the critical shear rate $\dot\gamma_c = 1/\lambda$. The values of the parameters corresponding to the different cases simulated in this work are given in Table 6.2. Throughout the rest of this paper, the fluid number will refer to this table and to the physical properties and rheological parameters reported therein.
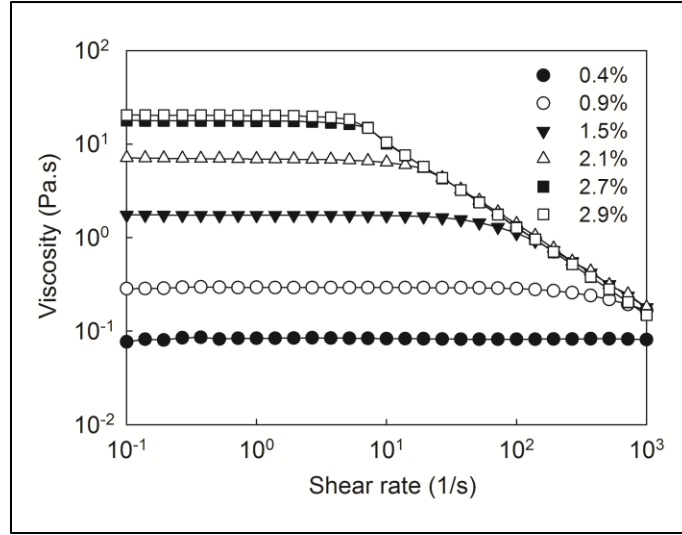
Figure 6.2: Shear viscosity data for aqueous solutions of Steol with different salt concentrations from 0.4 to 2.9 wt% (from [154])

In the case of the Newtonian fluids, the Reynolds number of a mixing system can be defined as $Re = \rho ND^2/\mu$, where ρ and μ are the density (in $Kg.m^{-3}$) and the viscosity of the fluid (in $Pa.s$), N is the rotational speed (in RPS) and D is the impeller diameter (in m). For a fluid obeying a Carreau-Yasuda model, the Reynolds number can be generalized through the concept of Metzner and Otto [31] as

$$Re_g = \frac{\rho ND^2}{\eta_\infty + (\eta_0 - \eta_\infty)[1 + (\lambda K_s N)^a]^{\frac{n-1}{a}}} \tag{6.2}$$

where K_s is the Metzner-Otto constant. In this work, its value is set at 15, as was proposed by [143] for a similarly low power law index ($n = 0.1$) and confirmed to be adequate in our previous experimental work [35, 154].

For impeller comparison purposes, the power consumption P (in W) can be characterized by two dimensionless characteristic numbers, N_p and K_p. The power number N_p, given by

$$N_p = P/\rho N^3 D^5 \tag{6.3}$$

is constant in the turbulent regime. Conversely, the power constant $K_p = N_p.Re$ is constant in the laminar regime and can be easily generalized to non-Newtonian fluids as $K_p = N_p.Re_g$.

The pumping capacity of a mixing system can also be represented by a dimensionless characteristic number, the axial flow number N_q, which is given by

$$N_q = Q_z^+/ND^3 \qquad (6.4)$$

where the axial pumping (or flow rate) Q_z^+ is computed as $Q_z^+ = \frac{1}{H}\int_V u_z^+ dv$, with H the fluid height (in m), V the total volume of the mixing system (in m^3) and u_z^+ the upward axial velocity (in $m.s^{-1}$), in other words, $u_z^+ = u_z$ if $u_z > 0$ and 0 otherwise. In the case of close-clearance impellers, the computation of the axial pumping is generally approximated by the flow crossing a set of horizontal planes [13, 36].

6.2.3.3 The lattice Boltzmann method

Only a brief presentation of the LBM is given here and the reader is referred to [58, 144] for further explanations on the method and [155] for more details on the implementation used in this work.

The lattice Boltzmann method (LBM) is a powerful numerical tool, which differs from other classical CFD methods by obtaining the solution of the Navier-Stokes equations from a simplified kinetic equation, the Boltzmann equation, based on the kinetic theory of gases. It has been successfully applied to the simulation of problems highly relevant for industrial applications, such as suspensions [72, 111, 139], turbulent flows [86, 117, 158], multiphase flows [159-161], non-Newtonian flows [16, 27, 54, 115] and porous media flows [3, 110, 115]. The main advantages of the LBM are its highly parallel efficiency, due to the locality of the computations and the regularity of the mesh, as well as its ability to handle for instance turbulence and rheologically complex fluids. The LBM simulates the macroscopic dynamics of a fluid by propagating and colliding fluid particles along the bonds of a lattice grid. The primary variable of the LBM is then a population of fluid particles.

Thus, at time t, for a lattice at position $\vec{x}$, populations $f_k(\vec{x}, t)$ are associated with velocity vectors $\vec{e}_k$, which are determined by the type of lattice. In this work, the D3Q15 lattice [63] is used and the velocity vectors are defined as

$$\vec{e}_k = \frac{\delta x}{\delta t} \begin{cases} 0 & k = 0 \\ (\pm 1,0,0), (0,\pm 1,0), (0,0,\pm 1) & k = 1-6 \\ (\pm 1,\pm 1,\pm 1) & k = 7-14 \end{cases} \tag{6.5}$$

The collision-propagation procedure can then be written (with the BGK [60, 63] collision operator) as follows

$$f_k(\vec{x} + \vec{e}_k \delta t, t + \delta t) - f_k(\vec{x}, t) = -\frac{1}{\tau} \left[f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t) \right] \tag{6.6}$$

where the equilibrium populations are computed as

$$f_k^{(eq)}(\vec{x}, t) = \omega_k \left[\rho + \rho_0 \left(\frac{\vec{e}_k \cdot \vec{u}}{c_s^2} + \frac{(\vec{e}_k \cdot \vec{u})^2}{2c_s^4} - \frac{\vec{u} \cdot \vec{u}}{2c_s^2} \right) \right] \tag{6.7}$$

with τ the relaxation parameter, $c_s = \frac{1}{\sqrt{3}} \frac{\delta x}{\delta t}$ the lattice speed of sound and ω_k the weights of the populations, defined as $\frac{2}{9}$ if $k = 0$, $\frac{1}{9}$ if $k = 1-6$ and $\frac{1}{72}$ if $k = 7-14$, for the D3Q15.

The macroscopic variables are computed in every lattice as

$$\rho(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t) \tag{6.8}$$

$$\rho_0 \vec{u}(\vec{x}, t) = \sum_{k=0}^{q-1} f_k(\vec{x}, t) \, \vec{e}_k \tag{6.9}$$

where $q = 15$ is the total number of populations per lattice and ρ_0 is the mean density of the fluid.

The viscosity of the fluid η is introduced into the method through the relaxation parameter

$$\tau = \frac{\eta}{\rho_0 \delta t c_s^2} + \frac{1}{2} \tag{6.10}$$

Thus, in the Newtonian case, the value of the relaxation parameter is constant in time and space, and is used to adjust the time step δt.

For non-Newtonian simulations, the value of the viscosity $\eta(\dot{\gamma})$ is given by a rheological model (the Carreau-Yasuda model in this work), so that the relaxation parameter is no longer constant. The shear rate tensor $\boldsymbol{S}$, used to compute the shear rate $\dot{\gamma} = \sqrt{2\boldsymbol{S}:\boldsymbol{S}}$, can be evaluated from the velocity field with a second-order centered formula. It can also be evaluated directly from the populations [62, 89]:

$$S_{ij}(\vec{x}, t) = -\frac{1}{2\tau\rho_0 c_s^2 \delta t}\sum_{k=0}^{q-1}\left(\vec{e}_{ki}\vec{e}_{kj} - \frac{\delta_{ij}}{D}\vec{e}_k.\vec{e}_k\right)f_k^{(neq)}(\vec{x}, t) \tag{6.11}$$

where D is the dimension of the problem, δ_{ij} is the Kronecker delta function and $f_k^{(neq)}$ the so-called non-equilibrium populations computed as $f_k^{(neq)}(\vec{x}, t) = f_k(\vec{x}, t) - f_k^{(eq)}(\vec{x}, t)$.

The latter technique is used in this work since it preserves the locality of the LBM and has shown to provide the same accuracy for Newtonian fluids [62, 155]. In the non-Newtonian case, the shear-rate tensor $\boldsymbol{S}$ is used to determine the relaxation parameter τ. It is evaluated through Eq. (6.11) using the previous time step: $\tau(\vec{x}, t - 1)$. This choice is justified by the desire to preserve the explicit form of the LBM scheme and to prevent the use of costly fixed-point iterations.

In conclusion, the LBM is based on an explicit scheme where all computations are simple and local. The scheme has proven to be second-order accurate in time [121, 140, 144, 145] and recovers the solution of the Navier Stokes equations under the hypotheses of small Mach and Knudsen numbers. With this method, these two numbers are defined as $Ma = \frac{|\vec{u}|}{c_s}$ and $Kn = \frac{\mu}{\rho L c_s}$, where L is a characteristic length. The impact of the limitation on the Mach number will be discussed in the next section.

6.2.3.4 Practical aspects of the simulation process

As the LBM uses Cartesian structured meshes, the discretization of the Maxblend impeller implies determining which lattice nodes are fluid and which ones are solid. To do so, a mesh is used to describe the geometry of this solid part. In addition, due to its rotation, the state of the lattices (solid or fluid) evolves with time. As the initialization of the new fluid lattices is non-trivial and may affect the accuracy of the results, we chose here to use the non-equilibrium corrected refill procedure [88] to accomplish this task. With this approach, the missing

populations are determined by extrapolation, thereby reducing errors on the flow field around the moving impeller. The reader is referred to [155] for detailed explanations. In this work, the lattice spacing δx was set to 1.77 mm, corresponding to a total close to 7 million lattices. This lattice spacing was observed to be fine enough to yield preliminary results with variations on the average velocity that are lower than 1%, when compared to the solutions obtained with finer lattices.

After the discretization process, boundary conditions have to be imposed between fluid and solid lattice nodes. Here, due to the complexity of the geometry, boundary conditions are a key aspect of the whole simulation process. The boundary conditions for the tank walls, the baffles and the Maxblend impeller are imposed with the Extrapolation method (EM) [78]. Owing to this approach, the accuracy of the LBM is conserved [78, 155] and the shape of the boundaries is precisely described. On the other hand, the free surface is approximated by a free slip boundary condition [58], and considered to be flat. This approximation is generally used to simplify the simulation process, as it prevents the need to simulate a two-phase flow (air and liquid). Here, the error generated by this simplification is insignificant considering that baffles largely reduce the height of the vortex, which in any case is small in the laminar regime.

For a given set of physical parameters (density ρ, viscosity η and rotational speed N or velocity $\vec{u}$) and a given lattice spacing δx, the last step of the simulation process is the selection of the relaxation parameter τ. Substituting the lattice speed of sound into Eq. (6.10) leads to:

$$\delta t = \frac{3\rho_0 \delta x^2 (\tau - 0.5)}{\eta} \tag{6.12}$$

and the Mach number becomes:

$$Ma = \frac{\sqrt{3}|\vec{u}|\delta t}{\delta x} \tag{6.13}$$

It appears from these two equations that the time step δt, the relaxation parameter τ and the Mach number are proportional. Given that the value of τ is constant in the Newtonian case, its selection is a compromise between accuracy (the smaller Ma the better) and computational time (not too small δt). In the case of high velocity $|\vec{u}|$ (high Re), δt must be small enough to guarantee a Mach number lower than 0.2, which has been observed for various problems to be

adequate in terms of numerical stability. This can be achieved by selecting a relaxation parameter close to 0.5, thereby drastically reducing the range of acceptable values of τ.

In the case of a non-Newtonian fluid, the value of the relaxation parameter τ is a function of the apparent viscosity $\eta(\dot{\gamma})$. In the case of a shear-thinning fluid ($n < 1$), the value of this viscosity is inversely proportional to the shear rate $\dot{\gamma}$, as deduced from Eq. (6.1). Moreover, Eq. (6.10) shows that the relaxation parameter τ and $\eta(\dot{\gamma})$ are proportional, so that τ will also decrease with an increase in the shear rate. In this case, the selection of the reference relaxation parameter $\tau_0 = \tau(\eta_0) = \tau\big(\eta(\dot{\gamma} = 0)\big)$ is crucial, as it must be high enough to account for the total variation of the viscosity in the computational domain during the simulation. In this work, as the fluid is strongly shear-thinning ($n = 0.05$), τ_0 was fixed at 4. In that the relaxation parameter τ and the Mach number are proportional (see Eqs. (6.12) and (6.13)), for a given value of δx (1.77 mm in this work), the velocity $\vec{u}$ must be small enough to ensure a small Mach number. Basically, the more the fluid is shear-thinning, the smaller the maximum achievable Reynolds number. Note that, for a given Mach number, the impact of the rheology on the computational time is negligible. In addition, preliminary tests in the case of the circular Couette flow with a power-law model have shown that the second-order accuracy of the LBM was conserved.

Our parallel implementation of the LBM is based on the use of the MPI library. All the computations were performed on Calcul Quebec Colosse supercomputer, the characteristics of which are given in Table 6.3.

Tableau 6.3: Characteristics of the Colosse supercomputer.

Number of nodes	960
Type of node	2 Intel Nehalem-Ep 4-core proc.
Total number of cores	7680
Memory per node	24 GB
Total available memory	23 TB
Network	Infiniband QDR (40 Gb/s)
Peak performance	88 Tflops

6.2.4 Simulation results

In this section, LBM simulations are presented for Newtonian and strongly shear-thinning fluids (Carreau-Yasuda model with $n = 0.05$). In order to validate the simulation process, results are first compared to experimental data and FEM results.

6.2.4.1 Newtonian flow

First, we focus on Newtonian results in order to validate the simulation process, as more results are available in the literature for this type of fluids. Our LBM results are compared with FEM results [13] and data from 2D PIV measurements [154] and the decolorization technique [35]. For the FEM simulations, an unstructured mesh of 290,336 $P_1^+ - P_0$ tetrahedral elements was used. The corresponding system of 2.12 million equations was solved by means of the Krylov-based Uzawa solver.

The LBM results are presented for Reynolds numbers up to 140, as our current LBM simulation procedure became numerically unstable for higher Re with $\delta x = 1.77$ mm. This limitation could be overcome by reducing the lattice spacing or using the MRT collision model [122] to improve the numerical stability. Nevertheless, going above $Re = 140$ was not deemed necessary within the scope of this work. The corresponding maximum Mach numbers were lower than 7.10^{-2} for all LBM simulation results, which is small enough to ensure a good accuracy. In addition, the total number of impeller revolutions required to achieve a periodic solution depends on the Reynolds number. For instance, at $Re = 2.1$, only 2 revolutions were necessary. Conversely, 12 revolutions were required for $Re = 140$. The average computational time for 1 revolution was around 3.5h with 48 cores.

6.2.4.1.1 Power and pumping curves

The N_p versus Re power curves, obtained from experimental data based on torque measurements [35], FEM results [13] and our LBM simulations are presented in Fig. 6.3(a). A good agreement can be noticed between the LBM and FEM results and the experimental data. First, in the laminar regime ($Re < \sim 70$), the slope is constant at -1, confirming that the power number is linearly proportional to the Reynolds number (i.e. $K_p = N_p \cdot Re = cst$). Next, for higher Reynolds numbers, a transition zone can be observed as the slope of the curve decreases.
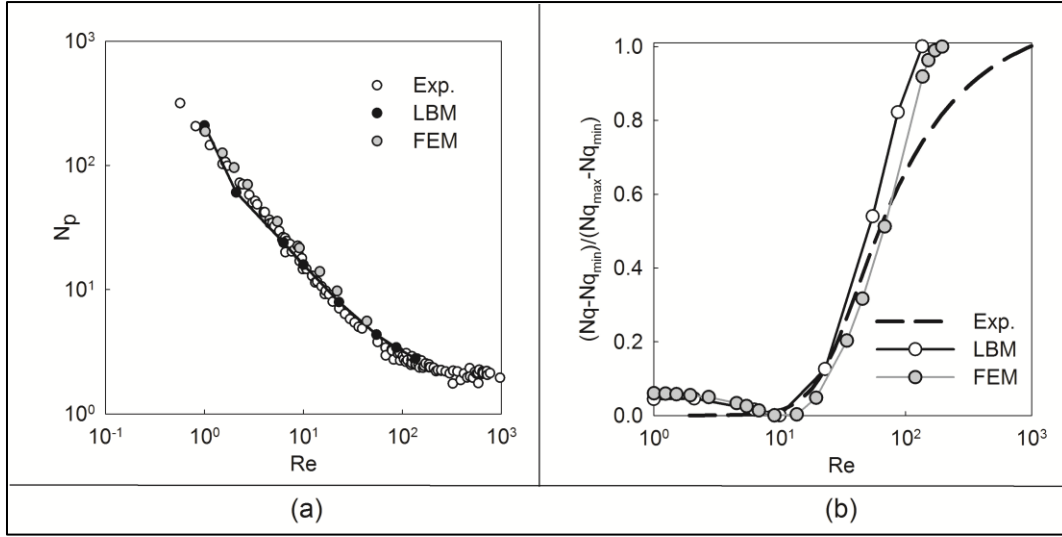
Figure 6.3: Power and pumping curves for the Maxblend mixing system in the Newtonian case with experimental data [35], FEM [13] and LBM results.

In the case of the pumping capacity, experimental measurements are generally more difficult to take, although recent approaches appear to be promising. For instance, the use of the decolorization method [32] has recently been extended to evaluate flow number N_q from the decolorization rate [35]. From this information, an estimate of the global pumping (radial, tangential and axial) is obtained. The value of the axial pumping is therefore overestimated, but the trend with respect to the Reynolds number has shown to comply with that obtained using other techniques.

In order to compare the axial pumping predicted by the LBM to the global pumping obtained from the decolorization method, it is then necessary to scale the results. To do so, a normalized flow number is introduced:

$$N_q^* = \frac{N_q - N_q^{min}}{N_q^{max} - N_q^{min}} \tag{6.14}$$

where N_q^{min} and N_q^{max} are the minimum and maximum flow numbers for the corresponding techniques.

Fig. 6.3(b) displays the variation of the normalized flow number N_q^* versus the Reynolds number from the decolorization method [35] as well as the FEM [13] and LBM results. A good agreement can be noticed between the two numerical approaches as the difference is generally

under 5%, except at Reynolds numbers close to 1 where the differences are closer to 10%. Comparisons with the experimental data are also good as the three curves exhibit the same trend: a small pumping capacity in the deep laminar regime ($Re < 10$), followed by a sharp increase in the transition regime up to $Re = 140$. However, the decolorization method is not accurate enough to describe the pumping efficiency in the deep laminar regime, let alone the slight increase predicted by both the LBM and FEM when $Re < 10$. The latter numerical results suggest that the axial flow may be different in this regime. The next section will investigate this aspect.

6.2.4.1.2 *Analysis of the flow field*

The flow generated by an impeller can be decomposed into two parts: the tangential component that follows the rotation of the impeller and the secondary flow, which is the sum of the axial (i.e. pumping) and radial contributions. As the distributive mixing mechanism is principally generated by the secondary flow, it has already been investigated experimentally and numerically in previous investigations focusing on the Maxblend [13, 154]. Recently, the 2D PIV was applied to investigate the effect of highly shear-thinning and viscoelastic fluids on the secondary flow [154]. These results revealed the dependence of the secondary flow patterns on the fluid rheology. However, one has to keep in mind that those measured values of the radial and axial components of the flow come from the projection of the flow field on a plane perpendicular to that goes through the impeller and the baffles. While it is known that perspective errors in 2D PIV can be significant [162], the data reported in [154] seemed to capture qualitatively well the flow fields at various Reynolds numbers.

Fig. 6.4 compares the secondary flows obtained with the results of the LBM, PIV [154] and FEM [13], for Reynolds numbers of 2, 23, 55 and 140. The vertical cross-sections are perpendicular to the impeller and represent only one half of the domain. It is important to mention that the magnitude of the secondary flow is different for the FEM results because they pertained to other viscosities and densities. In addition, the studied mixing system was comprised of 4 baffles rather than 2.
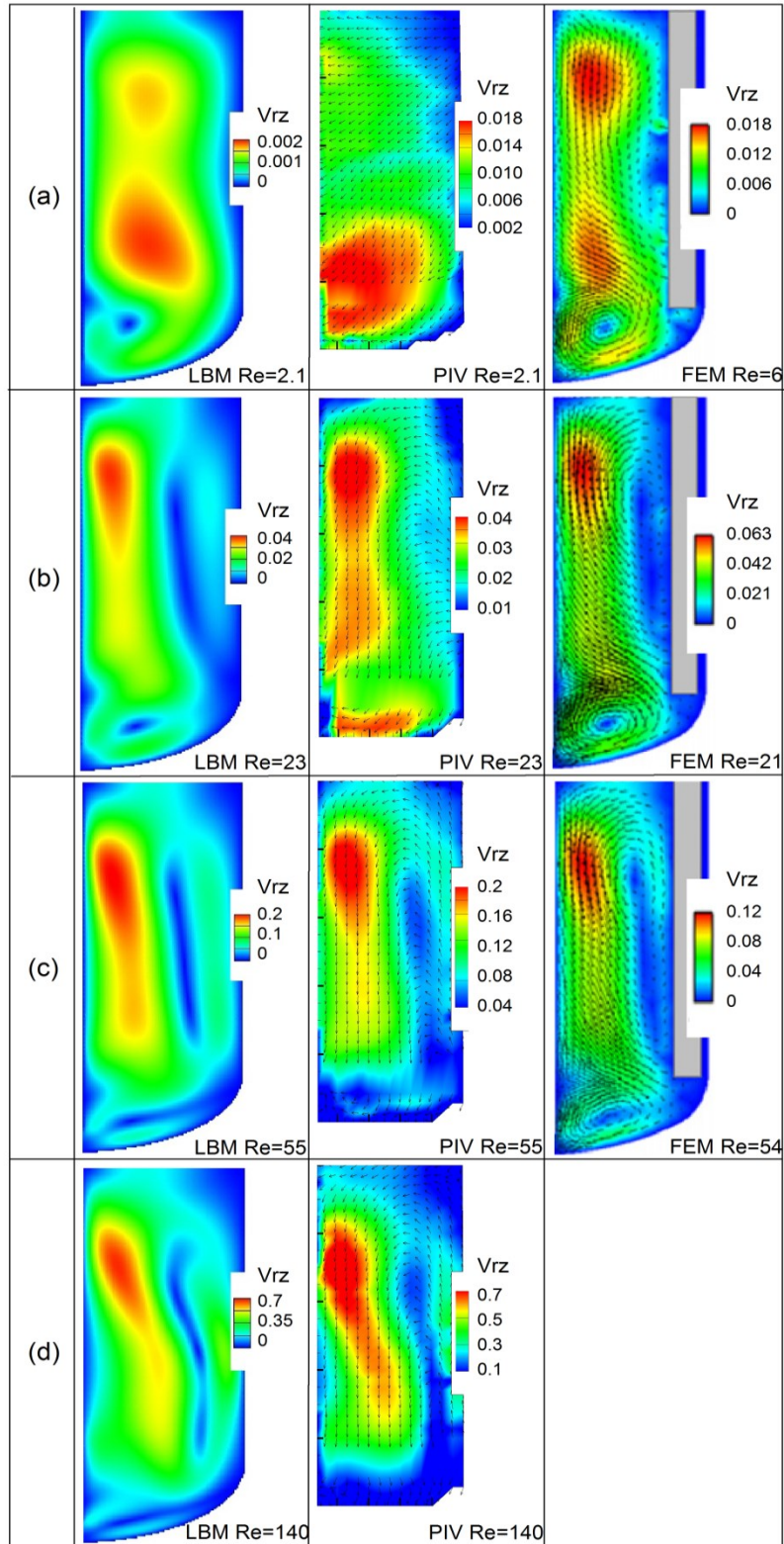
Figure 6.4: Magnitudes (Vrz) of the radial and axial components of the velocity for the Newtonian fluid obtained with the LBM, PIV [154] and FEM [13].

For Reynolds numbers between 23 and 140, Figs 6.4(b), (c) and (d) show a rather good agreement between the secondary flows obtained with the three approaches. These results are in accordance with previous works [13, 35, 36, 154], in that the shape of the secondary flow does not drastically change over this range of *Re*. More precisely, it is characterized by an intense downward flow around the impeller and a moderate upward flow near the tank walls, which is reminiscent of a toroidal shape. In addition, when comparing the 2D PIV and LBM results for the same configurations (density, viscosity and impeller speed), it appears that the magnitude of the maximum velocity obtained with both approaches are similar. In order to extend this analysis, Fig. 6.5 presents the profile of the dimensionless axial velocity $Vz/(\pi ND)$ with respect to the radius, at $z/H = 0.75$ for different Reynolds numbers from 6 to 55. Once again, a good agreement can be observed among the results obtained with the LBM, PIV [154] and FEM [13]. In particular, it confirms that the maximum axial velocities measured with the 2D PIV are close to the numerical results.
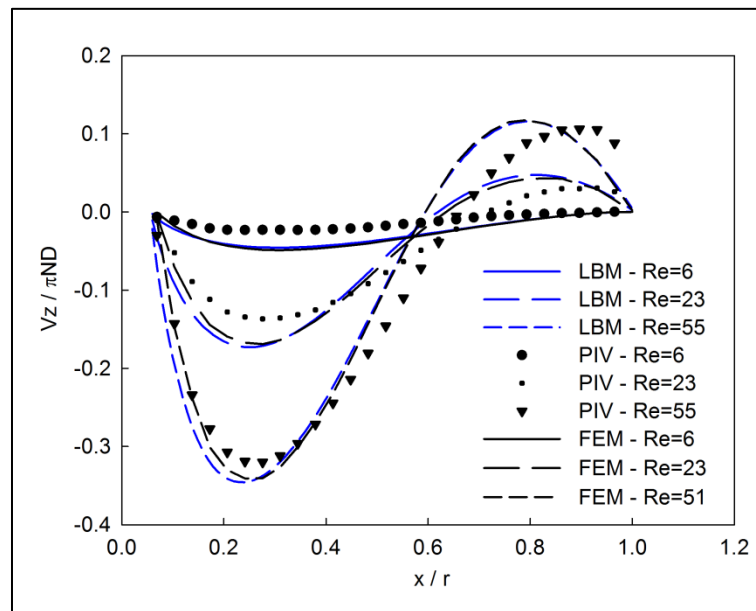
Figure 6.5: Dimensionless axial velocity profiles at z/H=0.75 with the LBM, PIV [154] and FEM [13].

In the case of the secondary flows obtained at $Re = 2$, Fig. 6.4(a) shows differences in the contours of the secondary flows obtained with the LBM, the FEM and the PIV. For instance, a good agreement can be noticed between the numerical results, although the upper part of the secondary flow is slightly underestimated by the LBM. We consider that the most likely

explanation for this lies in the difference in the Reynolds number (6 for the FEM and 2 for the LBM) and the differences in the mixing systems as mentioned before. Larger discrepancies can be noted with the 2D PIV contours. While similarities do exist between the PIV and LBM results regarding the shape of the flow, the magnitude of the maximum velocity is 9 times larger with the PIV. This is a priori surprising given that for other Reynolds numbers, the maximum velocities were similar for these two methods. We will return to this point in the next section.

From a broader perspective, the secondary flows obtained at $Re = 2$ with the LBM, the PIV and the FEM, suggest that the toroidal shape of the axial pumping volume observed at higher Re is not valid in the deep laminar regime. This result is compliant with conclusions drawn in the previous section, in that the pumping was not constant in the laminar regime (see Fig. 6.3(b)). Clearly, a better characterization of the secondary flow in the deep laminar regime can help understand the variation of the pumping efficiency found therein and the related mixing issues raised in previous works [13, 36, 154].

6.2.4.1.3   *Transition from the deep laminar to the transitional regimes*

In previous numerical and experimental studies [13, 154], the characterization of the secondary flow was limited to the visualization of sections perpendicular to the impeller. This choice can be easily explained by the difficulty to experimentally measure the flow in other positions, as the impeller then hides the view. However, we will show that resorting to only these cross-sections in the deep laminar regime may lead to inaccurate perceptions.

Fig. 6.6 displays the three-dimensional shape of the axial pumping volume obtained with the LBM, for Reynolds numbers of 2 and 23. In both cases, the negative values of the axial component of the velocity are in blue and the positive ones in red. Figs. 6.6(c) and 6.6(d) show the standard toroidal shape of the axial pumping volume generated by the Maxblend at $Re = 23$. As mentioned previously, the corresponding secondary axial and radial flow is composed of a downward component around the impeller and an upward component near the tank walls. Conversely, Figs. 6.6(a) and 6.6(b) show that the axial flow does not follow the same behavior at $Re = 2$. In fact, the fluid goes up in front of the rotating impeller and goes down behind. We believe this phenomenon is due to the predominance of the viscous forces, which prevent the formation of the shape observed at the higher value of Re. This is worthwhile mentioning since it is the first time that the secondary flow is shown to be completely different in the deep laminar

regime. It also explains why poor mixing performances have been reported in this regime [13, 36, 143, 154].
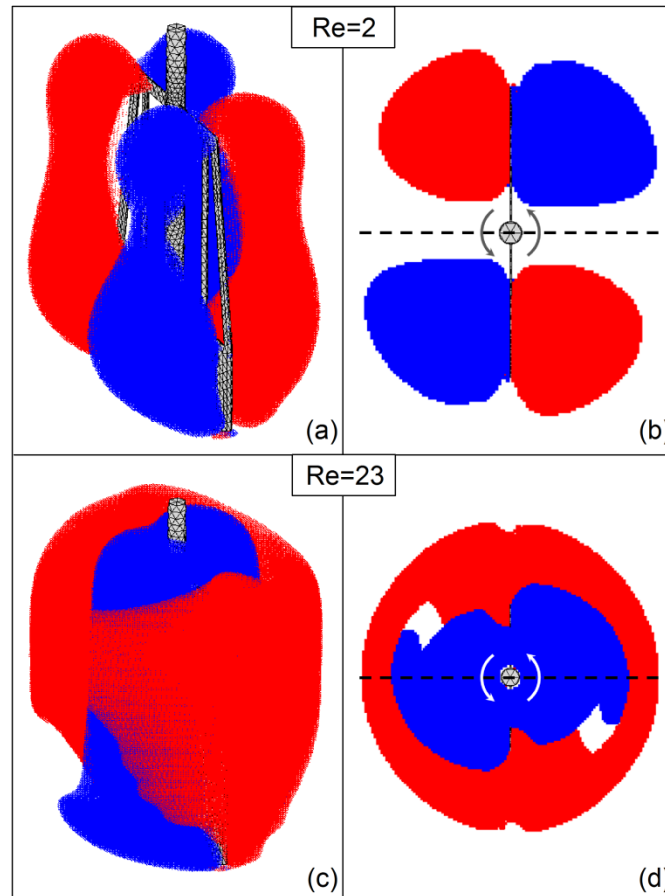
Figure 6.6: Axial pumping volumes of the Newtonian flow predicted with the LBM, at Reynolds numbers of 2 and 23: (a) and (c) correspond to three-dimensional views and (b) and (d) to top views. The red and blue colors denote positive and negative values of the axial component of the velocity, respectively. The dashed lines represent the section used for the PIV measurements, and the arrows indicate the sense of rotation.

Figs. 6.6(b) and (d) show top views of the axial pumping volumes at Reynolds numbers of 2 and 23, respectively. The dashed lines represent the section used for the 2D PIV measurements and the secondary flow fields in Fig. 6.4. Fig. 6.6(b) clearly shows that, at $Re = 2$, using such a section is inadequate to characterize the secondary flow in the tank, as the volumes are not axisymmetric and the absolute values of the velocities are very small. It explains why the 2D PIV fails to measure a precise maximum velocity in this case. Conversely, for higher Reynolds numbers, when the shape of the axial pumping volume is toroidal, the section perpendicular to

the impeller is adequate to characterize the secondary flow. These results illustrate that simulation can help set up the sections used for 2D PIV measurements. It also underlines the limitations of 2D flow visualization.

Knowing that the secondary flow is different in the laminar regime, it is then important to determine how it affects the pumping efficiency. Fig. 6.7 presents the variation of the relative importance of the three components of the time-averaged velocity. It appears from the curves that the radial component of the flow is rather small and constant (from 9.5 to 12%). Next, for the axial component, the curve can be decomposed into three parts: a rather small value (lower than 13%) in the deep laminar regime ($Re < 10$), followed by a linear increase in the laminar regime, and finally, a rather constant but large value (around 24%) for $Re > 80$. These results establish that the conversion of the tangential motion into pumping (or axial motion) is weak and minimum around $Re = 10$. This minimum corresponds to a state in between the two secondary flows depicted in Figs. 6.6(b) and (d). For higher Reynolds numbers (i.e. $Re > 10$), the conversion of the tangential motion into pumping increases, thereby indicating that in the case of a toroidal secondary flow (Figs. 6.6(c) and (d)), the increase of the inertial forces leads to enhanced pumping. The relative intensity of the axial flow seems to level off at around $Re = 80$.
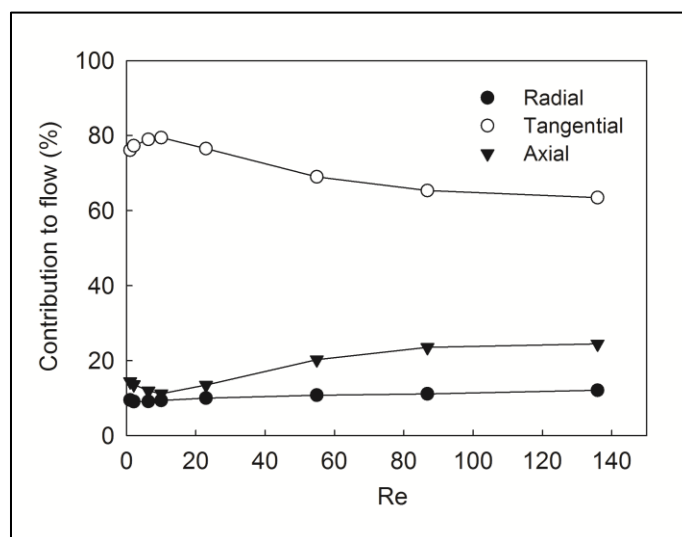
Figure 6.7: Variation of the relative importance of three components of the time-average mean velocity obtained with the LBM in the Newtonian case.

6.2.4.2 Strongly non-Newtonian flow

In this section, we extend our investigation to a strongly shear-thinning fluid, in order to evaluate the impact of the rheology on the pumping capacity of the Maxblend impeller. The maximum Mach numbers achieved were lower than 0.15, which is sufficiently small to ensure a reasonable accuracy. As the fluid is strongly shear-thinning ($n = 0.05$), a minimum viscosity of $\eta_\infty = \eta_0/250$ was set in order to prevent the occurrence of instabilities. Such strongly non-Newtonian fluids can be easily tackled with the LBM, but the reference relaxation parameter τ_0 must be cautiously chosen (see Section 6.2.3.4). Note that our FEM code was unable to simulate a power low index n lower than 0.3 [13].

Once again, the total number of impeller revolutions required to achieve a periodic solution depends on the generalized Reynolds number. Given that the rotational speeds are rather small, a maximum of 5 revolutions was necessary at a generalized Reynolds number Re_g of 55. The average computational time for 1 revolution was around 4h on 48 cores.

6.2.4.2.1 Power and pumping curves

Fig. 6.8(a) displays the power curves obtained with non-Newtonian LBM simulations (fluid no. 5 in Table 6.2) and experimental data [35] for Newtonian and non-Newtonian fluids. As suggested in [35], the use of the generalized Reynolds number Re_g, coupled with a Metzner-Otto constant of 15, allows to use the Newtonian power curve as a master curve. Furthermore, even if the fluid is strongly shear-thinning ($n = 0.05$), a good agreement is observed between LBM results and experimental data.

In addition, Fig. 6.8(b) shows the variation of the axial flow number N_q with respect to the Reynolds number (using fluids nos. 1, 2 and 5 presented in Table 6.2). Quite clearly, the pumping capacity of the Maxblend is largely affected by the rheology of the fluid. It is important to mention that this result is limited to the laminar and transitional regimes, as the pumping was recently shown to be independent of the rheology in the turbulent regime [35]. In the latter work, the occurrence of problematic flow patterns giving rise to two segregated regions in the tank were revealed by the decolorization method. As an illustration, Fig. 6.9 shows these two segregated zones for $Re_g = 8$. To gain insight into the effect of rheology on flow behavior in the laminar regime, the flow field of the strongly shear-thinning fluid is next analyzed.
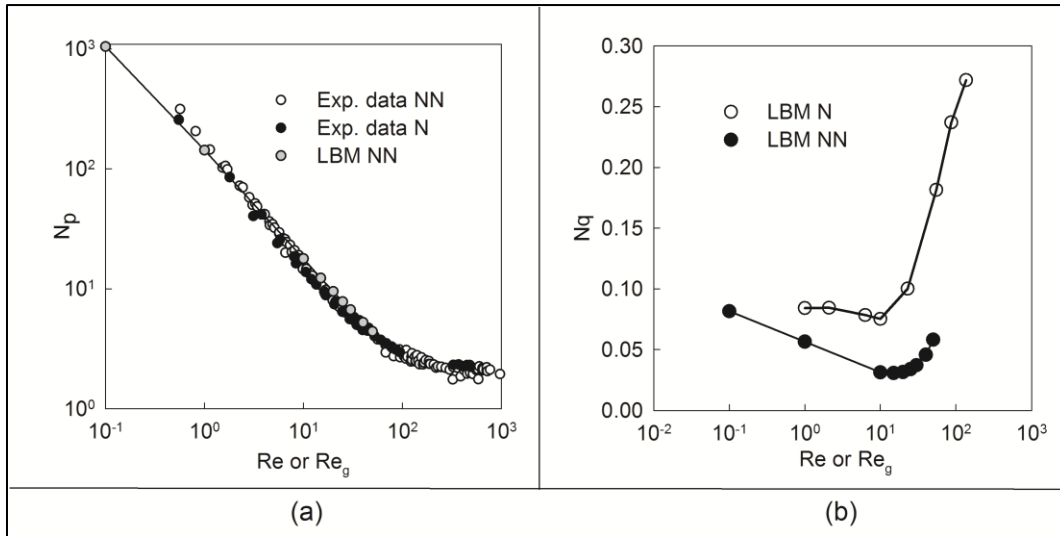
Figure 6.8: Power and pumping curves for the Maxblend mixing system: experimental data [35] and LBM results for the (N) Newtonian and (NN) non-Newtonian cases.
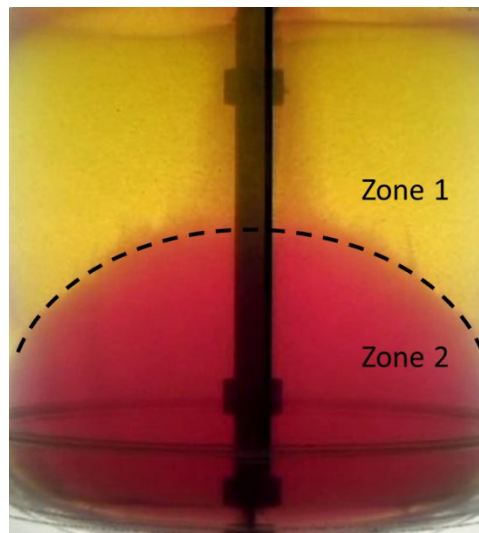
Figure 6.9: Segregation zones for $Re_g = 8$. Adapted from [35].

6.2.4.2.2 *Analysis of the flow field*

Fig. 6.10 compares the contours of the secondary flows obtained with the 2D PIV [154] and LBM, for generalized Reynolds numbers of 6 and 9, corresponding to fluids nos. 3 and 4, respectively (see Table 6.2). While the lower parts are rather similar in all cases, the upper parts of the contour plots exhibit different behaviors. In addition, the 2D PIV overestimates the

magnitude of the secondary flow (radial and axial components of the velocity), but the differences decrease with the increase in Re_g (from a factor of 10 at $Re_g = 6$ to 4 at $Re_g = 9$). It is noteworthy that the agreement between the LBM and PIV are not as good at low Re_g, as in this case, the absolute values of the measured velocities are too small to ensure a good accuracy, as discussed in Section 6.2.4.1.3. Similarly to the Newtonian results (see Fig. 6.6(b)), the position of the section used for the 2D PIV measurements is inadequate.
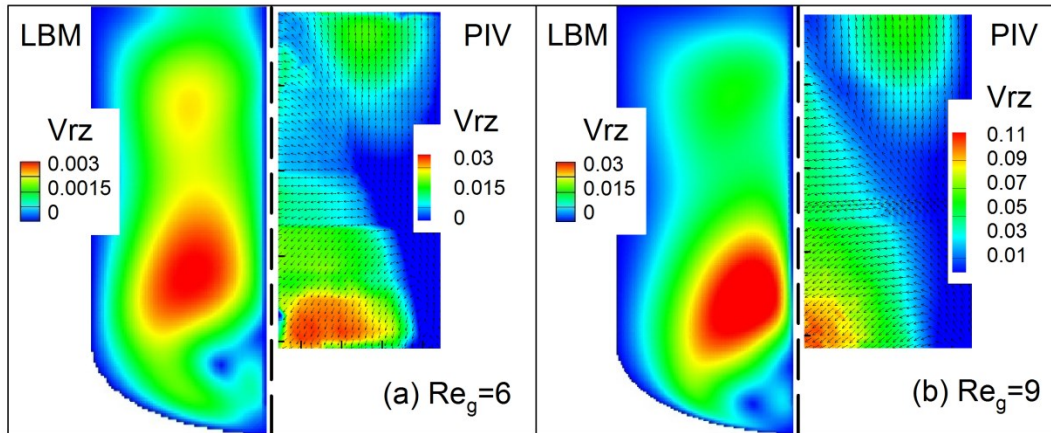
Figure 6.10: Magnitudes (Vrz) of the radial and axial components of the velocity for the strongly non-Newtonian fluid obtained with the LBM and PIV [154] for (a) $Re_g = 6$ (fluid 3) and (b) $Re_g = 9$ (fluid 4).

In summary, the LBM can be successfully used to characterize the secondary flow with strongly non-Newtonian fluids. However, with the current BGK collision model and a lattice spacing $\delta x = 1.77$ mm, the maximum Re_g that can be simulated is limited, as mentioned in Section 6.2.3.4. The 2D PIV remains a good alternative in the transitional and turbulent regimes, as it was shown to accurately determine the shape of the secondary flow as well as the maximum value of the axial velocity.

6.2.4.2.3   *Transition from the deep laminar to the transitional regimes*
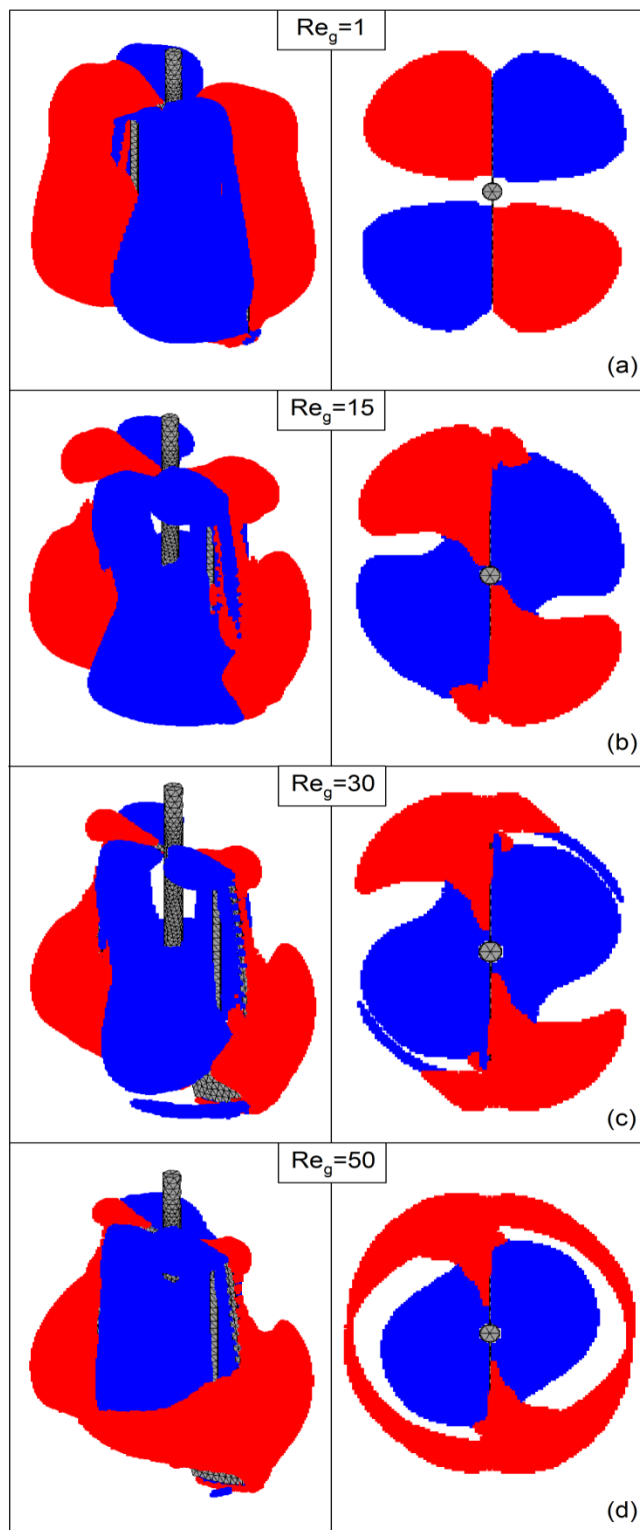
Figure 6.11: Axial pumping volumes of the strongly non-Newtonian flow predicted with the LBM at Re_g of (a) 1, (b) 15, (c) 30 and (d) 50. The red and the blue colors denote positive and negative values of the axial component of the velocity, respectively.

Simulations up to $Re_g = 55$ were achieved using fluid no. 5 (see Table. 6.2) to investigate the variation of the pumping efficiency with respect to Re_g. Three-dimensional shapes of the axial pumping volume obtained with the LBM are presented in Fig. 6.11, which correspond to generalized Reynolds numbers of 1, 15, 30 and 50, respectively. In both cases, the negative values of the axial component of the velocity are in blue and the positive ones in red. Fig. 6.11(a) shows that the axial flow at $Re_g = 1$ is rather similar to the one observed at $Re = 2$, in the Newtonian case. This flow is characterized by an upward component in front of the rotating impeller and a downward component behind. The similarity with the Newtonian case implies that, in the entire domain, the local shear rate is lower than the critical shear rate ($\dot{\gamma}_c = 1/\lambda$) of the fluid. With the increase of Re_g, it can be observed in Figs. 6.11(b-d) that the shape of the axial pumping volume is significantly modified. Similarly to the results for the Newtonian fluid, the fluid flows downward around the impeller and upward near the tank walls. However, contrary to the Newtonian case, the pumping in the upper part of the mixer is much weaker compared to the one at the bottom. It shows that, in case of a strongly non-Newtonian fluid, even if the paddle (located at the bottom) is able to generate pumping, the grid (located at the top) fails to conserve it. In order to determine if this lack of pumping around the grid can be related to the problematic flow patterns observed experimentally at $Re_g = 8$ [35] (see Fig. 6.9), the variation of the apparent viscosity in the tank is analyzed.

Fig. 6.12 gives the maps of the viscosity obtained with the LBM, for Reynolds numbers of 1, 15, 30 and 50. The vertical cross sections are perpendicular to the impeller and the baffles. Fig. 6.12(a) confirms that, at $Re_g = 1$, the shear rate is globally under the critical value of the fluid, as the viscosity is hardly affected by the motion of the impeller. In fact, the bottom of the tank is the only area where the viscosity decreases, as the shear rate is maximal in the small clearance between the impeller and the tank. For higher generalized Reynolds numbers, as shown in Fig. 6.12(b-d), an envelope of small viscosities develops, above which the viscosity becomes rapidly large and within which a number of isolated large viscosity islands can be noticed. These results are relevant as the shape of the top of the envelope is similar to the interface between the segregated zones observed in Fig. 6.9. In addition, as the viscosity at the top of the tank is high for every Reynolds number, it shows that even if the paddle does impart rather large shear rates at the bottom of the tank, the upper part of this paddle and the grid are unable to do so. As a matter

of fact, this phenomenon is reduced with an increase of the generalized Reynolds number, as the size of the islands diminishes and the envelope occupies more and more space in the tank.
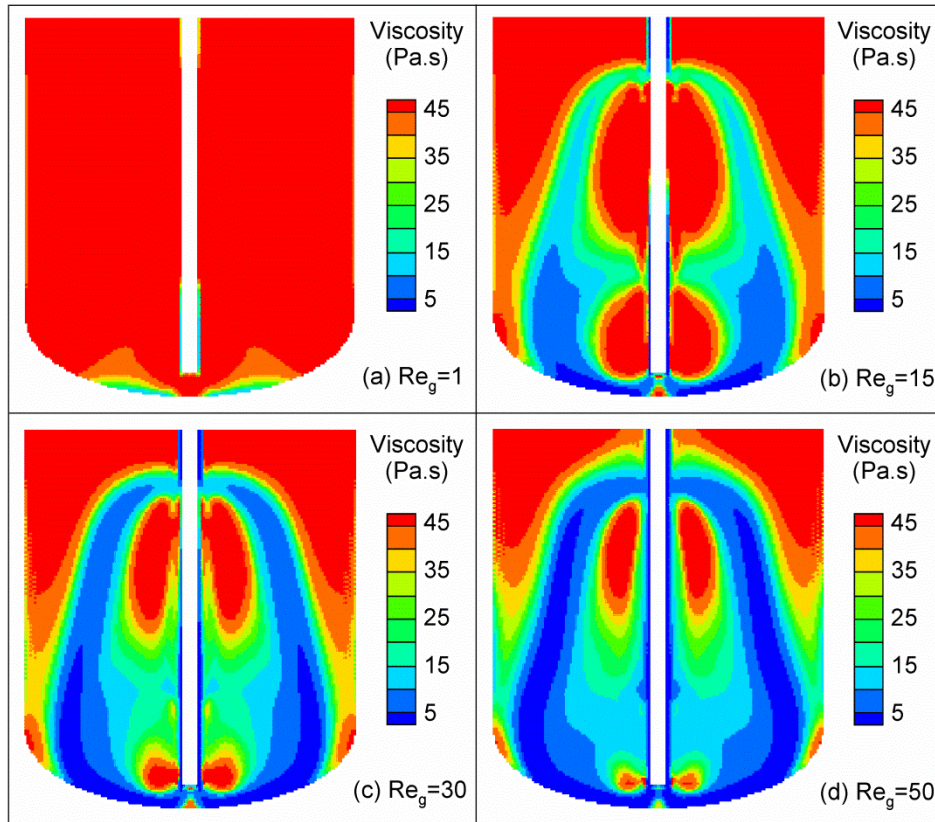
Figure 6.12: Viscosity maps obtained with the LBM for the strongly non-Newtonian fluid at Re_g of 1, 15, 30 and 50.

As a complement, Fig. 6.13(a) presents the variation of the relative importance of the three components of the time-average mean velocity with respect to the generalized Reynolds number. It shows that the radial and axial components are both small (always lower than 13%) for all Re_g. It suggests that, in this range of generalized Reynolds numbers, increasing the inertia forces does not create more pumping. Fig. 6.13(b) compares the axial components of the time-average mean velocity for the Newtonian and highly shear-thinning fluids (from Figs. 6.7 and 6.13(a)). It appears that the pumping of the strongly non-Newtonian fluid is weaker. Moreover, the Reynolds number corresponding to the minimum value of the axial component is slightly larger (20 as opposed to 10), which is close to 15, the value at which the volume of the islands was maximum in Fig. 6.12. For complex mixing applications, it is important to determine efficient operating conditions. The curves in Fig. 6.13 imply that, in the case of a strongly non-Newtonian fluid, a

range of Reynolds numbers (from $Re_g = 10$ to 30) larger than that for a Newtonian fluid (from $Re_g = 5$ to 15) should be avoided to prevent mixing problems.

(a)   (b)
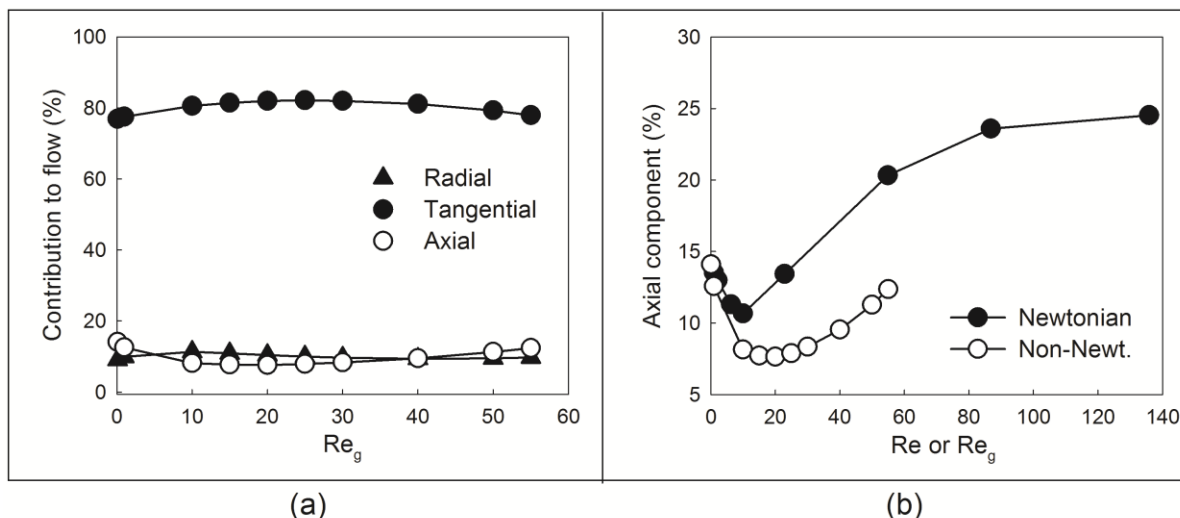
Figure 6.13: (a) Variation of the relative importance of the three components of the time-average mean flow for the non-Newtonian case and (b) comparison of the axial components for the Newtonian and non-Newtonian fluids.

6.2.5 Conclusions

The objective of the work was to shed light on the pumping generated by the Maxblend impeller for Newtonian and strongly non-Newtonian fluids. To do so, LBM results were first compared to previous FEM simulations [13] in the Newtonian case. These results were also used to explain recent experimental data based on 2D PIV [154] and the decolorization method [35]. In particular, the importance of the section used for the 2D PIV measurements was underlined. In the case of a strongly non-Newtonian fluid ($n = 0.05$), the LBM was shown to be efficient in so far as it was able to simulate the flow of this type of fluid contrary to our finite element code.

First, in the Newtonian case, we showed that the LBM results are in good agreement with the FEM results and the experimental data. From this comparison, it was noticed that the pumping capacity of the Maxblend impeller is highly affected by the Reynolds number. Thanks to three-dimensional visualizations, the variation of the pumping efficiency in the laminar regime was related to a change of structure in the secondary flow. In fact, in the deep laminar regime, the axial flow is characterized by an upward component in front of the rotating impeller and a

downward component behind. This suggests that, under a critical Reynolds value ($Re \approx 10$), the inertia is too small to transform the tangential flow into pumping. In the case of strongly non-Newtonian fluid flows, the same type of transition from radial to axial flow was observed in the laminar regime. However, contrary to the Newtonian flow, a lack of pumping was noticed in the upper part of the impeller. Finally, the presence of an envelope of small viscosities was underlined and related to the creation of two segregated zones that have been observed experimentally [35].

6.2.6 Acknowledgments

6.3 Résultats complémentaires

Les résultats présentés dans cette section ont pour but de vérifier les propriétés de convergence spatiale du schéma LBM dans le cas de fluides non newtoniens. Pour ce faire, nous allons étudier à nouveau l'écoulement de Couette cylindrique. Dans cette section, les conditions aux limites sur la hauteur sont périodiques (voir section 5.2.4.1) et le nombre de Reynolds vaut 1. La rhéologie du liquide est modélisée par la loi de puissance $\eta = m\dot{\gamma}^{n-1}$, avec $m = 1$. Dans ce cas, les solutions analytiques en vitesse, en taux de cisaillement et en puissance sont :

$$u_\theta(r) = \omega \frac{(r_{in}r_{out})^{2/n}}{\left(r_{out}^{2/n} - r_{in}^{2/n}\right)}\left(\frac{1}{r^{2n-1}} - \frac{r}{r_{out}^{2/n}}\right) \tag{6.15}$$

$$\|\dot{\gamma}\| = \frac{2\sqrt{2}\omega}{n}\frac{(r_{in}r_{out})^{2/n}}{\left(r_{out}^{2/n} - r_{in}^{2/n}\right)}\frac{1}{r^{2/n}} \tag{6.16}$$

$$P = m\pi h n \left(\frac{2\omega}{n}\right)^{(n+1)}\frac{(r_{in}r_{out})^2}{\left(r_{out}^{2/n} - r_{in}^{2/n}\right)^n} \tag{6.17}$$

La figure 6.14 présente ainsi les erreurs sur (a) la vitesse et (b) le taux de cisaillement en fonction de la taille de lattice, pour des indices de puissance de 0.2, 0.4, 1 (newtonien) et 1.4. Il ressort de la figure 6.14(a) que si la valeur de l'indice de puissance n'affecte pas l'ordre de précision en vitesse, les erreurs augmentent lorsque n diminue. La conservation de l'ordre 2 de précision n'est pas surprenante puisque le modèle rhéologique n'affecte pas le développement mathématique du passage de Boltzmann à Navier-Stokes [14], présenté dans la section 2.1. La conservation de l'ordre 2 en vitesse a d'ailleurs déjà été soulignée par Boyd [15] pour un modèle de loi de puissance. De la même manière, la figure 6.14(b) montre que la valeur de l'indice de puissance n'affecte pas l'ordre 2 de précision du taux de cisaillement et que les erreurs augmentent lorsque n diminue. On notera quand même que la stabilité numérique est plus sensible à la rhéologie puisque, pour la taille de lattice la plus petite, les simulations ne convergent pas pour $n = 0.2$.
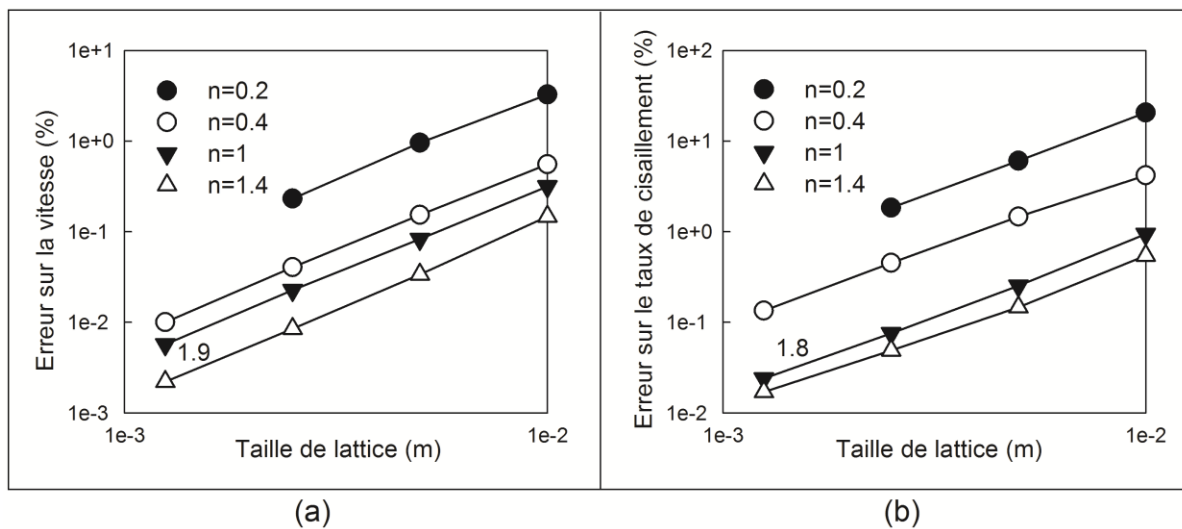
Figure 6.14: Impact de l'indice de puissance n sur la précision de (a) la vitesse et (b) du taux de cisaillement pour le problème de Couette.

Il est aussi important de vérifier l'impact de la rhéologie sur la précision de la prédiction de consommation de puissance. Ainsi, la figure 6.15 présente les erreurs sur la puissance, calculées à partir (a) du taux de cisaillement et (b) du couple (voir Section 5.2.3.2), pour des indices de puissance de 0.2, 0.4, 1 (newtonien) et 1.4. Pour la puissance calculée à partir du couple (figure 6.15(b)), on observe un comportement similaire à celui observé pour la vitesse et le taux de cisaillement, c'est-à-dire un ordre de précision proche de 2 et une augmentation de l'erreur lorsque n diminue. Dans le cas de la puissance calculée à partir du taux de cisaillement (figure

6.15(a)), comme mentionné dans la Section 5.2.4.1, l'erreur sur la puissance ne diminue pas forcément avec la taille de lattice.
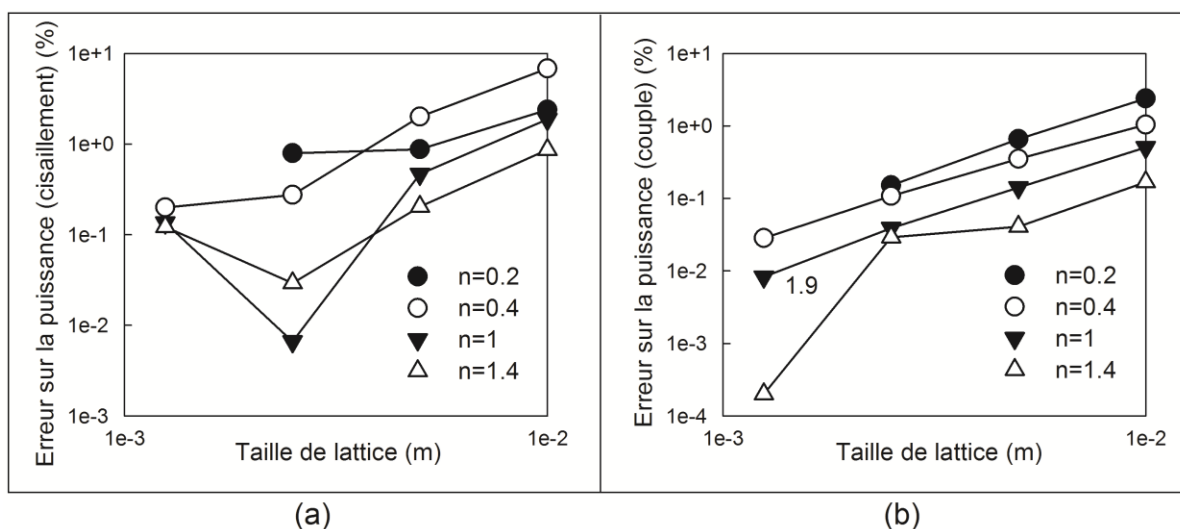
Figure 6.15: Impact de l'indice de puissance n sur la puissance calculée à partir (a) du taux de cisaillement et (b) du couple pour le problème de Couette.

CHAPITRE 7   DISCUSSION GÉNÉRALE

Les écoulements visqueux sont caractérisés par une forte résistance à l'écoulement, ce qui empêche la création de tous phénomènes turbulents. Un des exemples les plus classiques concerne les écoulements dans les milieux poreux, caractérisés par une surface de contact importante et de géométrie complexe. Dans le cas général, la forme de l'écoulement n'est pas seulement liée à la géométrie du problème, elle est aussi fortement affectée par la rhéologie du fluide. Ces problématiques sont encore plus importantes dans le cas des écoulements polyphasiques. En effet, à la géométrie du problème s'ajoutent celles des frontières qui séparent les phases. La forme de l'écoulement n'est plus seulement affectée par les propriétés des différentes phases, mais aussi par leurs interactions. Dans cette thèse, nous nous sommes intéressés plus particulièrement au cas des écoulements monophasiques visqueux en cuves agitées.

Les mélangeurs spécialisés pour les liquides visqueux sont caractérisés par des géométries complexes, nécessaires à l'homogénéisation du mélange en l'absence de turbulence. Dans le cas des mélangeurs discontinus, les pales doivent racler la cuve afin de prévenir la stagnation du produit près des parois. La performance d'un système de mélange est alors associée à sa capacité à disperser et à distribuer, ces grandeurs étant quantifiées à partir de la consommation de puissance et de la création de pompage. Si les performances sont largement dépendantes de la géométrie des pales et des cuves, la rhéologie de la mixture joue aussi un rôle prépondérant.

En complément des méthodes expérimentales, l'utilisation des méthodes numériques permet d'améliorer la compréhension des écoulements visqueux en cuves agitées. Afin de prédire adéquatement l'hydrodynamique au sein d'un système de mélange spécialisé pour les liquides visqueux, l'interaction entre le liquide et la pale doit être précisément modélisée. Autrement dit, la méthode numérique doit permettre un traitement précis de la géométrie, des parties mobiles et de la rhéologie du liquide. La littérature montre que c'est principalement la méthode des éléments finis qui est utilisée dans ce cas. La problématique de la complexité de la géométrie est généralement traitée par une méthode de conditions aux limites immergées. Comme les modèles rhéologiques viennent perturber le système d'équations obtenu, la majorité des résultats concerne des écoulements monophasiques dont les propriétés rhéologiques ne sont pas fortement non newtoniennes ($n > 0.3$). En conclusion, les choix de modélisation sont généralement basés sur

un compromis entre la complexité et les temps de calcul, ce qui limite le passage à l'étude d'écoulements polyphasiques ou à rhéologies complexes. Il est alors pertinent de tester d'autres méthodes numériques afin de dépasser ces limitations. Ainsi, l'objectif de cette thèse était de développer une méthode de Boltzmann sur réseau efficace pour la simulation des écoulements visqueux en cuves agitées.

La méthode de Boltzmann sur réseau (LBM) est une approche récente, basée sur la théorie cinétique des gaz. L'utilisation de l'échelle mésoscopique permet de modéliser la dynamique d'un fluide à partir du comportement d'un groupe de particules imaginaires. De cette manière, la solution des équations de Navier-Stokes est obtenue par l'application d'un schéma explicite, basé sur des calculs simples et locaux. Associé à un maillage structuré cartésien, la méthode est hautement parallèlisable et permet l'utilisation d'un très grand nombre d'éléments ou de cellules (lattices). La vision mésoscopique du fluide facilite l'intégration de phénomènes microscopiques comme la rhéologie, mais présente aussi certains désavantages. En effet, l'utilisation d'une variable primaire mésoscopique complique l'imposition de grandeurs macroscopiques, ce qui rend difficile l'imposition de conditions aux limites et l'initialisation des lattices.

Les différentes applications de la LBM dans la littérature permettent de tirer plusieurs conclusions. Tout d'abord, les simulations d'écoulements dans les milieux poreux montrent que la LBM permet de traiter un niveau de complexité géométrique difficilement atteignable avec les méthodes classiques de la CFD. Ensuite, pour des écoulements simples avec des solutions analytiques, plusieurs études montrent la sensibilité de la précision à la définition des conditions aux limites. De la même manière, l'initialisation des lattices peut affecter la précision, notamment autour des géométries avec parties mobiles. Finalement, les résultats pour des systèmes de mélange comprenant des turbines Rushton prouvent que la LBM est efficace pour la simulation du mélange en régime turbulent. Ils montrent aussi que l'intégration de modèles rhéologiques et d'approches Euler-Lagrange, comme les méthodes de particules discrètes (DPM), est réalisable dans des petits systèmes de mélange. Ces conclusions ont permis de définir trois objectifs spécifiques reliés à l'applicabilité de la LBM aux écoulements visqueux en cuves agitées.

Le premier objectif spécifique était de comparer les différentes stratégies pour l'imposition des conditions aux limites en LBM. Cette étape est très importante puisque le mélange visqueux est généré par l'interaction entre la pale et la cuve, ce qui nécessite une modélisation précise de leurs

effets sur le fluide. Cependant, l'utilisation d'une variable primaire mésoscopique complique l'imposition de grandeurs macroscopiques comme la vitesse de l'obstacle. Il est donc très important de comparer les précisions qui peuvent être obtenues avec les stratégies proposées dans la littérature. Pour ce faire, trois stratégies ont été sélectionnées parmi les approches applicables aux géométries complexes : La méthode du rebond modifié (MBB), la méthode d'extrapolation (EM) et la méthode de conditions aux limites immergées pour la LBM (IB-LBM). Chacune de ces stratégies est représentative d'une classe de conditions aux limites possédant les mêmes caractéristiques. Ainsi, la stratégie MBB est la plus simple car elle approxime les frontières courbes par des profils en escalier. La stratégie EM utilise la distance à la paroi pour extrapoler les populations aux nœuds solides. Finalement, la stratégie IB-LBM utilise des points de contrôle pour contraindre la vitesse des nœuds environnants.

Dans l'article 1, les comparaisons ont été effectuées sur des géométries fixes sans partie mobile, afin d'éviter les erreurs associées à l'initialisation des nœuds nouvellement fluides qui apparaitraient atour d'un obstacle en mouvement. Tout d'abord, la simulation de l'écoulement de Couette cylindrique a permis de vérifier que seule la stratégie EM est capable de conserver la précision du deuxième ordre pour la convergence spatiale de la vitesse. Dans le cas des stratégies MBB et IB-LBM, la précision chute au premier ordre. Cette perte de précision globale est due à la création d'erreurs importantes près des frontières, plus particulièrement à celles où sont imposées des vitesses non nulles. La simulation de l'écoulement de Couette cylindrique a aussi permis d'étudier la sensibilité de la précision aux paramètres numériques des stratégies EM et IB-LBM. Dans le cas de la stratégie EM, il ressort que l'impact des coefficients d'extrapolation est négligeable et que leur optimisation n'est pas essentielle. De la même manière, l'introduction d'une erreur sur le calcul des distances n'affecte pas significativement la précision globale. À l'inverse, la précision des résultats obtenus avec la stratégie IB-LBM est très sensible à la répartition des points de contrôle. Il ressort que la variabilité des résultats peut être importante pour une petite variation du nombre ou de la position des points de contrôle. Finalement, il a été montré que les stratégies d'imposition de conditions aux limites affectent aussi la stabilité numérique. Plus précisément, la stratégie IB-LBM ne permet pas d'atteindre des nombre de Mach supérieurs à 0.1, tandis que les stratégies MBB et EM sont numériquement stables jusqu'à 0.3.

La comparaison des stratégies d'imposition de conditions aux limites a ensuite été étendue à des systèmes de mélange comprenant une ancre et un Paravisc. Afin d'éviter les erreurs associées à

l'initialisation des nœuds nouvellement fluides, les simulations ont été effectuées dans un repère Lagrangien fixé sur la pale. Les stratégies ont été comparées sur les prédictions de consommation de puissance et de capacité de pompage. Les résultats sur la consommation de puissance montrent que les stratégies MBB et EM donnent des résultats très similaires, proches des valeurs disponibles dans la littérature. De plus, la diminution de la taille des lattices permet d'observer une convergence vers une valeur fixe, proche des données expérimentales. Notons que, les résultats obtenus avec la stratégie IB-LBM sont différents de ceux obtenus avec MBB et EM, mais restent acceptables. Les résultats sur la capacité de pompage permettent de compléter la comparaison puisqu'ils confirment une proximité des prédictions obtenues avec les stratégies MBB et EM. À l'inverse, la stratégie IB-LBM donne des résultats inférieurs, avec une variabilité conséquente en fonction de la taille de lattice. En conclusion, dans le cas des mélangeurs raclants, il semble que l'utilisation de la stratégie IB-LBM ne permet pas d'obtenir le même degré de précision qu'avec les deux autres approches. L'observation des champs de vitesse montre que si l'écoulement global est bien représenté, des perturbations apparaissent aux alentours de la pale, ce qui peut générer des erreurs locales importantes sur la vitesse. Il est aussi important de noter que la proximité des résultats obtenus avec les stratégies MBB et EM est plutôt surprenante, puisqu'elles présentaient des précisions différentes sur l'écoulement de Couette cylindrique. Pour autant, la comparaison reste partielle puisqu'elle ne concerne que des grandeurs globales. Il est donc possible que l'étude d'autres aspects souligne des différences notables entre les deux stratégies. Dans le cas des mélangeurs industriels, il serait intéressant d'étudier l'impact des stratégies sur des configurations présentant des zones mortes, afin d'étudier les prédictions sur leurs positions et leurs tailles. Une autre possibilité serait de quantifier l'impact des stratégies sur le calcul de trajectoire de particules. Finalement, la comparaison des profils de pression pourrait compléter la compréhension de l'influence des stratégies sur l'écoulement global.

Le deuxième objectif spécifique était de déterminer la précision de la LBM dans le cas de géométries complexes. Suite aux conclusions de l'article 1, la stratégie d'imposition de conditions aux limites EM a été choisie pour sa précision. Elle possède aussi l'avantage d'évaluer précisément la position des frontières, ce qui est crucial pour la modélisation du mouvement d'une partie mobile. De plus, elle permet d'étudier l'impact d'une petite variation de la géométrie, ce qui est nécessaire à l'optimisation géométrique des procédés de mélange.

L'article 2 présente ainsi une étude approfondie de la précision du schéma LBM, couplé avec la stratégie EM, dans le cas de géométries complexes avec et sans parties mobiles. Tout d'abord, la simulation de l'écoulement de Couette cylindrique a permis d'étudier la précision du schéma pour la norme du taux de cisaillement. Cette caractérisation est importante puisque le taux de cisaillement est utilisé dans le calcul de la puissance consommée et interviendra dans les modèles rhéologiques étudiés dans la dernière partie de cette thèse. Il ressort que le schéma LBM possède une précision du deuxième ordre pour la convergence spatiale de la norme du taux de cisaillement. Cependant, une modification mineure des conditions aux limites peut entrainer une chute au premier ordre. Cette perte de précision globale semble être générée par des perturbations apparaissant dans les configurations géométriques où la stratégie EM n'est pas parfaitement définie. Cela confirme que dans le cas d'une géométrie non triviale, aucune stratégie d'imposition de conditions aux limites n'est parfaite en LBM. Si la précision en vitesse est bien contrôlée avec les méthodes de type interpolation ou extrapolation, des perturbations peuvent affecter la conservation de la masse ou la précision sur le taux de cisaillement. Afin de compléter l'étude du Couette cylindrique, deux approches possibles pour calculer la puissance ont aussi été comparées. Il ressort que la puissance calculée à partir du couple sur l'obstacle (intégrale surfacique) est plus précise que celle basée sur le taux de cisaillement (intégrale volumique). Cette différence s'explique par une mauvaise évaluation du volume total du fluide, due à l'utilisation d'un maillage structuré cartésien. En effet, lorsque la puissance est calculée à partir de l'intégrale volumique du taux de cisaillement, l'erreur sur la puissance est dominée par l'erreur sur le volume.

L'étude de la précision du schéma LBM a ensuite été étendue à la simulation de l'hydrodynamique d'un système de mélange Maxblend. Ce mélangeur a été sélectionné car il est performant sur une large gamme de nombres de Reynolds. La précision a été déterminée sur les prédictions de consommation de puissance et de capacité de pompage. Tout d'abord, à l'aide d'un repère Lagrangien fixé sur la pale, la configuration sans contre-pale a été simulée pour différents nombres de Reynolds. Les valeurs sélectionnées sont représentatives des conditions d'utilisation standards de ce système de mélange dans les régimes laminaire et transitoire. Les résultats obtenus montrent que les consommations de puissance et les capacités de pompage sont en accord avec les valeurs disponibles dans la littérature. De plus, la variation des performances en fonction de l'écart entre la pale et le fond de la cuve est aussi en accord avec les études

précédentes. Comme la stratégie EM permet d'étudier facilement cet aspect, une étude exhaustive de l'impact de l'espacement a été réalisée. De cette manière, il a été montré que si l'écart standard entre la pale et la cuve est proche de l'optimal en régime laminaire, un écart deux fois plus important serait plus performant en régime transitoire. Cette étude montre que, dans le cas de géométries sans partie mobile, la précision du schéma LBM permet de réaliser de l'optimisation géométrique de procédés.

Dans la dernière partie de l'article 2, la précision de la LBM a été étudiée dans le cas de géométries avec des parties mobiles. Pour ce faire, les configurations avec et sans contre-pales ont été simulées dans le repère naturel (eulérien du laboratoire). De cette manière, il est possible de quantifier les erreurs associées à la modélisation de l'impact de la pale en rotation sur le fluide. Dans un premier temps, en se basant sur les prédictions obtenues avec le repère Lagrangien, la précision des résultats sans contre-pale a été étudiée. Il ressort que les prédictions de consommation de puissance oscillent significativement dans le temps, ces oscillations étant dues aux initialisations de lattices nouvellement fluides, apparaissant après le passage de la pale. Cependant, les valeurs moyennes de consommation de puissance sont en accord avec les résultats précédents et l'amplitude des oscillations diminue lorsque la taille de lattice est réduite. Afin de compléter l'étude, les configurations avec contre-pales ont aussi été simulées. Dans ce cas, les résultats montrent que l'accroissement de puissance dû à la présence des contre-pales est en accord avec les données de la littérature. De la même manière, la variation de puissance maximale pendant une rotation de pale est proche de la valeur obtenue dans une étude numérique précédente utilisant la méthode des éléments finis (FEM). En conclusion, il ressort que, dans le cas de géométries complexes avec et sans parties mobiles, la LBM permet d'obtenir des prédictions précises de consommation de puissance et de capacité de pompage. Il est même possible de réaliser une optimisation géométrique d'un système de mélange, ce qui peut être plus fastidieux avec d'autres approches numériques qui nécessiteraient la génération d'un grand nombre de maillages. Dans le cas des géométries avec parties mobiles, il serait intéressant de compléter cette étude en utilisant la stratégie d'imposition de conditions aux limites IB-LBM. En effet, avec cette stratégie, la modélisation du mouvement d'un obstacle se limite à déplacer les points de contrôle et aucune initialisation de lattice n'est nécessaire. La comparaison des résultats avec la stratégie EM permettrait d'apporter un complément d'information à la comparaison des stratégies.

Le troisième objectif spécifique était d'étudier l'applicabilité de la LBM pour des rhéologies complexes inélastiques. Dans le cas du schéma LBM, l'utilisation d'un modèle rhéologique se limite à une modification locale du facteur de relaxation. Puisque cette intégration est aisée et ne perturbe pas significativement la précision ou les temps de calcul, il est important de déterminer les limites atteignables en termes de complexité rhéologique.

L'article 3 présente ainsi l'étude de l'impact de la rhéologie sur les mécanismes associés à la création du pompage dans le système de mélange Maxblend. La stratégie de simulation est basée sur les conclusions des deux articles précédents. Ainsi, dans le but de maximiser la précision sur la vitesse et sur le taux de cisaillement local, les conditions aux limites ont été imposées à l'aide de la stratégie EM. De la même manière, puisque les simulations avec des parties mobiles ont montré un niveau de précision suffisant, il est possible de simuler la configuration avec contre-pales, la plus couramment utilisée dans l'industrie. Tout d'abord, afin de définir une référence, l'évolution de la capacité de pompage en fonction du régime d'écoulement a été caractérisée dans le cas d'un liquide newtonien. Cette étape montre que les prédictions sont en accord avec les données expérimentales et numériques disponibles dans la littérature. Du point de vue de l'hydrodynamique, il ressort une différence structurelle de l'écoulement secondaire (composantes radiales et axiales) entre le régime laminaire profond et les régimes plus élevés. Cette étape a aussi permis de revisiter des résultats expérimentaux récents, ainsi que d'expliquer l'origine de certaines incohérences dans les mesures réalisées à faibles nombres de Reynolds.

L'étude a ensuite été étendue à la simulation d'un liquide fortement rhéofluidifiant (indice de puissance de 0.05) modélisé à l'aide d'un modèle de Carreau-Yasuda. Le choix du modèle rhéologique est motivé par deux études expérimentales récentes qui montrent des patrons d'écoulements problématiques avec ce liquide. Plus précisément, dans le régime laminaire, les résultats expérimentaux ont souligné la présence de zones mortes volumineuses. Il est important de souligner qu'un modèle aussi fortement rhéofluidifiant serait très difficile à simuler avec d'autres méthodes CFD, comme celle des éléments finis. Après avoir vérifié que les prédictions de consommation de puissance étaient en accord avec les valeurs expérimentales, l'évolution de l'hydrodynamique en fonction du régime d'écoulement a été étudiée avec la LBM. Les résultats ont montré que, sur une certaine plage de vitesses de rotation, des zones avec de fortes disparités de viscosité apparente se créent. La forme de ces zones étant assez proche des observations expérimentales, cela pourrait expliquer les patrons d'écoulements problématiques. Cela montre

aussi que la LBM est adéquate pour l'étude de problèmes industriels comportant des rhéologies complexes.

Cette étude a aussi permis de déterminer les limitations associées à l'utilisation de la LBM dans le cas de rhéologies fortement rhéofluidifiantes. En effet, comme la variation de viscosité dans le volume est intégrée au travers du facteur de relaxation, il est nécessaire de pouvoir utiliser une plage importante de ce paramètre. Autrement dit, le paramètre de relaxation initial, correspondant à la viscosité maximale, doit être assez grand pour que la viscosité minimale obtenue n'entraine pas une valeur de relaxation trop petite (i.e. trop proche de 0.5) et donc instable pour le schéma LBM. D'un point de vue pratique, plus le modèle est rhéofluidifiant, plus le paramètre de relaxation de référence doit être important. Cependant, l'augmentation du nombre de Reynolds (et donc de la vitesse de rotation) nécessite de réduire le facteur de relaxation pour conserver la stabilité numérique et la précision de la méthode. Il ressort que l'utilisation de modèles fortement rhéofluidifiants entraine une limitation sur les nombres de Reynolds simulables. Par exemple, dans le cadre de l'article 3, avec une taille de lattice de 1.77 mm, il n'a pas été possible de dépasser une valeur de 60 pour le nombre de Reynolds généralisé. L'avantage est que, lorsque les simulations sont possibles, les temps de calcul restent semblables à ceux des cas newtoniens. Afin de dépasser les limitations sur les nombres de Reynolds simulables, il serait intéressant de tester d'autres modèles d'opérateur de collision. Par exemple, il est possible que l'utilisation d'un schéma avec plusieurs facteurs de relaxation (comme la MRT) permette d'améliorer la stabilité des calculs pour de faibles valeurs du facteur de relaxation (proches de 0.5).

CONCLUSION ET RECOMMANDATIONS

L'objectif principal de cette thèse était de développer une méthode de Boltzmann sur réseau (LBM) efficace pour la simulation des écoulements visqueux en cuves agitées. Pour ce faire, trois articles ont été présentés.

La simulation des procédés industriels de mélange visqueux est caractérisée par la difficulté à traiter la complexité de la géométrie, à intégrer la rhéologie de la mixture ainsi qu'à modéliser l'interaction entre les différentes phases. La plupart des travaux de recherche dans ce domaine se concentrent sur la modélisation, avec des méthodes classiques, de l'impact des pales sur le fluide et sur l'intégration des modèles rhéologiques. Comme les temps de calcul sont très importants, la majorité des études concernent des écoulements monophasiques dont les propriétés rhéologiques ne sont pas fortement non newtoniennes. Afin de dépasser ces limitations, il est intéressant d'étudier les possibilités offertes par d'autres méthodes numériques. Le travail présenté dans cette thèse a permis d'apporter une contribution à ce champ de recherche.

Tout d'abord, la comparaison de trois stratégies d'imposition de conditions aux limites a permis d'étudier leur impact sur le précision du schéma LBM ainsi que leur applicabilité à la simulation de systèmes de mélange. L'étude de l'écoulement de Couette cylindrique a permis de montrer que seule une stratégie basée sur l'interpolation ou l'extrapolation est capable de conserver la précision naturelle du schéma LBM pour la vitesse. À l'inverse, les autres approches génèrent des oscillations sur les vitesses aux alentours des frontières. L'étude des paramètres numériques associés à chaque stratégie a montré que seule la stratégie basée sur une condition aux limites immergées est sensible aux paramètres numériques. En effet, la disposition des points de contrôle, utilisés pour modéliser l'impact de la partie en rotation, affecte largement l'erreur sur la solution numérique. La comparaison a ensuite été étendue à la simulation de systèmes de mélange comprenant une ancre et un Paravisc. Il ressort que les prédictions de consommation de puissance et de capacité de pompage sont similaires avec l'approche la plus simple, la méthode du rebond modifié (MBB), ou avec l'utilisation d'une méthode d'extrapolation. Dans le cas de la stratégie de conditions aux limites immergées, les résultats sont proches mais présentent une variabilité conséquente en fonction de la taille de lattice. Il ressort que, dans le cas des mélangeurs raclants, cette stratégie ne permet pas d'obtenir la même précision, à cause de

l'apparition de perturbations sur la vitesse dans la zone de la pale. En conclusion, les stratégies d'interpolation ou d'extrapolation sont les mieux adaptées car elles permettent de minimiser les erreurs et prendre en compte de petites variations de la géométrie.

La deuxième partie de la thèse présentait une étude plus approfondie de la précision du schéma LBM, couplé avec la stratégie d'extrapolation, dans le cas de géométries avec et sans parties mobiles. L'étude de la précision sur la norme du taux de cisaillement a montré que cette grandeur est plus sensible que la vitesse à la définition des conditions aux limites, confirmant que même les stratégies les plus précises d'imposition de conditions aux limites perturbent le schéma LBM. De plus, les différentes méthodes disponibles pour calculer la puissance présentent des précisions différentes en fonction de la stratégie de simulation, c'est-à-dire avec ou sans parties mobiles. D'un point de vue plus général, la simulation du système de mélange Maxblend, dans les configurations avec et sans contre-pales, a permis de conclure que la LBM peut être efficacement utilisée pour simuler ce type de système de mélange. En effet, dans le cas d'une géométrie sans partie mobile (utilisation du repère lagrangien), la méthode a pu être utilisée pour étudier l'impact de l'espacement entre la pale et la cuve, montrant ainsi la possibilité de faire de l'optimisation géométrique avec cette approche. Dans le cas des géométries avec parties mobiles, les prédictions de consommations de puissance présentent des valeurs moyennes en accord avec les données de la littérature. Notons que l'initialisation des lattices nouvellement fluides, requise après le passage d'un objet, perturbe le champ de vitesse autour de la pale. Cependant, l'amplitude de ces oscillations diminue avec la taille de lattices.

La dernière partie de la thèse traite de l'applicabilité de la LBM pour des rhéologies complexes inélastiques. Comme l'intégration d'un modèle rhéologique dans le schéma LBM peut se faire d'une manière simple, qui n'affecte pas significativement la précision ou les temps de calcul, les limites atteignables avec un liquide fortement rhéofluidifiant (indice de puissance de 0.05) ont été étudiées. Pour ce faire, la caractérisation de l'écoulement secondaire (composantes axiales et radiales de l'écoulement) a permis de souligner les limites sur les nombres de Reynolds simulables pour une taille de lattice donnée. En effet, comme l'introduction du modèle de rhéologie se fait à travers le paramètre de relaxation, celui-ci doit représenter la variation totale de viscosité. Cependant, pour des raisons de stabilité, l'augmentation de la vitesse de rotation nécessite une réduction du paramètre de relaxation, ce qui limite la plage de nombres de Reynolds simulables pour une taille de lattice donnée. Malgré ces limitations, la méthode LBM a

pu être utilisée pour investiguer un problème industriel relatif à l'utilisation d'une rhéologie complexe.

En conclusion, la méthode de Boltzmann sur réseau a été utilisée avec succès pour la simulation de l'agitation d'écoulements monophasiques visqueux dans des systèmes de mélange. Les capacités et les limites pour le traitement de la complexité de la géométrie et de la rhéologie ont été caractérisées. S'il est certain que cette méthode ne va pas remplacer les méthodes des éléments et des volumes finis, elle peut être utilisée à bon escient dans certaines configurations. Par exemple, elle constitue une piste sérieuse pour tenter de simuler des écoulements polyphasiques ou à rhéologies complexes à l'échelle industrielle. Afin de continuer ce travail de recherche, les recommandations suivantes sont proposées :

1. Le raffinement local de maillage étant particulièrement adapté aux géométries des mélangeurs raclants (présence d'un entrefer), son application devrait permettre des gains de précision et de temps de calcul conséquents. Une automatisation de ce processus serait requise pour le traitement des parties mobiles.

2. Il serait intéressant d'étendre la comparaison des stratégies d'imposition de conditions aux limites à des écoulements comprenant des parties mobiles. Il est probable que les avantages des approches basés sur des conditions aux limites immergées ressortent plus clairement.

3. Il serait intéressant de déterminer les limites atteignables pour d'autres types de phénomènes rhéologiques. Par exemple, il faudrait quantifier l'impact de l'introduction des effets d'élasticité ou de thixotropie sur les possibilités du schéma LBM. Comme cette étape nécessite l'ajout d'une équation supplémentaire, il serait pertinent de comparer les différentes approches.

4. Puisque les méthodes de types particules discrètes (DPM) ont été appliquées avec succès à la LBM, il serait intéressant de voir dans quelles mesures cette méthode permet de recréer les viscosités apparentes de suspensions. Une attention particulière devra être portée sur le couplage solide-liquide.

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ANNEXE A – Intégration de LBGK sur l'espace des vitesses

Commençons par définir la moyenne d'un observable $\mathcal{A}(\vec{x}, \vec{e}, t)$ sur l'espace des vitesses $\vec{e}$ comme :

$$\langle \mathcal{A} \rangle (\vec{x}, t) = \frac{1}{\rho} \int \mathcal{A} f d\vec{e} \tag{A.1}$$

Si l'on multiplie l'équation (2.5) par $\mathcal{A}(\vec{x}, \vec{e}, t)$ et qu'on l'intègre sur l'espace des vitesses, on obtient :

$$\partial_t \rho \langle \mathcal{A} \rangle + \nabla. (\rho \langle \vec{e} \mathcal{A} \rangle) = -\frac{1}{\tau} (\langle \mathcal{A} \rangle - \langle \mathcal{A} \rangle^{eq}) \tag{A.2}$$

avec

$$\langle \mathcal{A} \rangle^{eq} = \frac{1}{\rho} \int \mathcal{A} f^{(eq)} d\vec{e} \tag{A.3}$$

Pour $\mathcal{A} = 1$, l'équation (A.2) devient

$$\partial_t \rho + \nabla. (\rho \vec{u}) = 0 \tag{A.4}$$

De même, pour $\mathcal{A} = \vec{e}$, l'équation (A.2) devient

$$\partial_t (\rho \vec{u}) + \nabla. \langle \vec{e} \vec{e} \rangle = 0 \tag{A.5}$$

Si l'on définit le tenseur des contraintes $\boldsymbol{\sigma}$ comme:

$$\boldsymbol{\sigma} = - \int f (\vec{e} - \vec{u})(\vec{e} - \vec{u}) d\vec{e} \tag{A.6}$$

l'équation (A.5) devient:

$$\partial_t (\rho \vec{u}) + \nabla. (\rho \vec{u} \vec{u}) - \nabla. \boldsymbol{\sigma} = 0 \tag{A.7}$$

Comme la trace du tenseur $\boldsymbol{\sigma}$ est :

$$tr(\boldsymbol{\sigma}) = \frac{2\rho\epsilon}{3} \tag{A.8}$$

le théorème de l'équipartition de l'énergie permet d'écrire la loi des gaz parfaits :

$$p = \rho\theta \tag{A.9}$$

avec p la pression hydrostatique et $\theta = k_B T/m$.

ANNEXE B – La décomposition de Chapman-Enskog

Commençons par rappeler l'équation LBGK (2.5) présentée dans la section 2 :

$$(\partial_t + \vec{e}.\nabla)f(\vec{x},\vec{e},t) = -\frac{1}{\tau}\Big(f(\vec{x},\vec{e},t) - f^{(eq)}(\vec{x},\vec{e},t)\Big) \tag{B.1}$$

La décomposition de Chapman-Enskog est basée sur une décomposition des phénomènes en fonction de leur échelle de temps. Dans cette procédure, la dérivée temporelle est décomposée comme :

$$\partial_t = \epsilon\partial_{t_0} + \epsilon^2\partial_{t_1} + \mathcal{O}(\epsilon^3) \tag{B.2}$$

De la même manière, les populations deviennent :

$$f = f^{(0)} + \epsilon f^{(1)} + \mathcal{O}(\epsilon^2) \tag{B.3}$$

À l'inverse, la dérivée spatiale n'est pas décomposée, c'est-à-dire $\nabla = \epsilon\nabla$.

Le paramètre $\epsilon \ll 1$ est généralement identifié comme étant le nombre de Knudsen K_n.

Lorsque cette décomposition est appliquée à l'ensemble des termes de l'équation (B.1), il est possible de les regrouper en fonction de leur ordre en ϵ. Pour les ordres 0 et 1, on obtient :

$$f^{(0)} = f^{(eq)} \tag{B.4}$$

$$(\partial_t + \vec{e}.\nabla)f^{(0)} = -\frac{1}{\tau}f^{(1)} \tag{B.5}$$