过渡流搅拌槽内固-液悬浮的直接数值模拟

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摘要 采用格子玻尔兹曼方法(lattice Boltzmann method), 研究了过渡流搅拌槽内颗粒悬浮过程的流体力学特征. 模拟中搅拌槽为平底方槽, 搅拌桨采用下压式45°四斜叶桨, 搅拌雷诺数 $Re=1334$, 属于过渡流; 颗粒体积分率最高达到8%. 本模拟解析了包括颗粒周围和颗粒间流动的搅拌槽内整个流场, 从而实现了在颗粒尺度上对颗粒-流体相互作用的研究. 同时, 本文也研究了体积分率、相位角对液相平均速度、液相湍流动能等流体力学特征值的影响规律. 结果表明, 随着搅拌槽内颗粒体积固含率的增加, 液相平均速度和液相湍流动能均衰减.

关键词 颗粒悬浮, 过渡流, 搅拌槽, 颗粒解析, 格子玻尔兹曼方法

固-液搅拌是很多工业生产过程中的重要操作单元, 例如制药工程、冶金、催化反应、结晶过程以及污水处理等. 在这些操作中, 流体通常处于层流^[1]或湍流状态^[2], 然而在反应器的放大、缩小过程中流体也会处于过渡流状态, 因此近年来研究者^[3,4]开始重视对于过渡流搅拌槽内流体力学特征规律的研究. 与单一液相搅拌相比, 颗粒和流体间存在动力学耦合作用使得固-液两相搅拌变得更为复杂, 同时这种耦合作用对搅拌槽内动量传递、质量传递、热量传递以及化学反应过程均有显著的影响. 因此研究过渡流搅拌槽内颗粒悬浮过程具有非常重要的意义.

关于搅拌槽内颗粒悬浮过程的研究进展, 本文将从实验和数值模拟两个方面进行介绍. 实验方面, Zwietering^[5]第一次提出临界悬浮转速的概念: 没有颗粒静止停留在搅拌槽槽底超过1~2 s条件下的搅拌转速. 基于此准则, 其他研究者^[6-8]针对不同搅拌几何结构、不同流动状况将临界悬浮转速进行了扩展, 并测量了搅拌过程的能耗、固体颗粒云高等全局流体力学特性. 随着流场测量技术的不断发展, 研究者逐

渐开始重视固-液搅拌槽内局部流体力学特性的研究. Unadkat等人^[9]、Montante等人^[10]和Guiraud等人^[11]采用粒子图像测速技术(particle image velocimetry, PIV)测量并研究了不同条件下固-液搅拌槽内的液相平均速度、液相脉动速度等流场信息. 然而当应用PIV技术于固-液两相体系中时, 固体颗粒的存在会阻挡、散射激光, 这种散射现象随着颗粒分率的增加而变得严重, 从而使得测量结果产生较大误差. 因此, 在这些研究中^[9-11], 颗粒体积固含率均被控制在1%以内. 为了解决这一问题, Li等人^[2,4]将折射率匹配技术应用到固-液两相搅拌槽中. Li等人^[2]将苯基硅油(折射率 $n=1.461$, $T=21^\circ\text{C}$)作为连续相, 石英玻璃球($n=1.460$, $T=21^\circ\text{C}$)作为分散相, 采用PIV技术进行固-液搅拌槽内颗粒分布、液相流场等流体力学特性方面的研究, 并首次将颗粒体积分率提高至8%.

数值模拟方面, 按照对分散相处理方法的不同, 可将固-液两相体系的研究分为欧拉-欧拉方法(Eulerian-Eulerian, E-E)和欧拉-拉格朗日方法(Eulerian-Lagrangian, E-L)两类. 在E-E方法中, 固相、液相均

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被视作连续介质；在E-L方法中，液相被视作连续介质而固相为被追踪的离散介质。本文将采用E-L方法进行搅拌槽内颗粒悬浮过程的数值模拟研究，因此接下来将主要介绍E-L方法中对于连续相和分散相的不同处理方式。对于连续相的处理，相比于雷诺平均N-S方法(Reynolds averaged Navier-Stokes, RANS)，大涡模拟(large eddy simulation, LES)和直接数值模拟(direct numerical simulation, DNS)求解尺度宽，结果更准确。这样，在颗粒追踪过程中，与RANS相比，LES减少了对随机模型的依赖，而DNS则无需这类模型。格子玻尔兹曼(lattice Boltzmann, LB)方法满足Navier-Stokes方程，可直接模拟流体运动，近年来在复杂流动模拟方面应用较广^[12]。在搅拌槽内流场模拟方面，LB方法具有边界条件容易处理、数值稳定性好、并行效率高等显著优势^[13]，因此本文采用LB方法求解液相流场。根据对分散相颗粒解析程度的不同，可将其分为点颗粒(point-particle)方法和解析颗粒(resolved-particle)方法两类。在很多采用点颗粒方法的研究中^[14-16]，没有考虑颗粒体积和颗粒间相互作用，然而随着固含率的增加，这些因素会对模拟结果产生很大的影响，因此这种方法通常只适用于颗粒固含率较低的体系。在此基础上，Derksen^[17]采用体积平均N-S方法(volume-averaged Navier-Stokes)并在模拟中设置了碰撞模型和曳力校正，从而可以得到颗粒体积和颗粒间相互作用力，进而实现了将点颗粒方法应用到高固含率体系当中^[17,18]。固-液搅拌的主要目的之一是为了加强颗粒和液体间的接触，因此研究发生在颗粒尺度下的流体力学特性是非常重要的。研究者^[1,4,19]采用LB方法对包括颗粒周围流场和颗粒间流场在内的搅拌槽内整个流场进行解析，实现了在颗粒尺度上对颗粒与其周围流场相互作用的研究。与点颗粒方法相比，解析颗粒方法的一个优势在于其不再需要曳力系数、传质系数等经验参数的设置。综上所述，本文将基于E-L方法进行过渡流搅拌槽内颗粒悬浮过程的直接数值模拟，利用LB方法处理连续相，采用解析颗粒方法来处理分散相。同时本文也对比分析了不同固含率、不同相位角条件下的数值模拟结果，这些数据对于将来相关实验研究具有重要的参考、对比价值。

1 数值模拟体系与方法

本文采用Somers和Eggels^[20,21]提出的LB方法来

求解液相流场。该方法中格子为均一的正方体，格子间距 Δ 和时间步长 Δt 分别用来表示模拟中空间和时间上的单位。模拟中搅拌槽、搅拌桨的几何结构如图1所示，搅拌槽为平底方槽，槽底边长(T)和槽高(H)均为264 Δ ，搅拌桨为下压式45°四斜叶桨(pitched blade turbine, PBT)，桨叶直径 $D=189.6 \Delta$ ，桨叶宽 $W=38.4 \Delta$ ，搅拌桨离底距离 $C=0.2T$ 。搅拌雷诺数 $Re \equiv ND^2/\nu=1334$ ，处于过渡区，其中 N 为搅拌转速， D 为桨叶直径， ν 为流体运动黏度。模拟中颗粒为粒径均一的球形颗粒，颗粒直径 $d_p=9.6 \Delta$ 。搅拌桨旋转1圈所需时间为6120 Δt 。本文在相位角 $\theta=30^\circ$ 时，在颗粒体积分数 $\Phi=0\%, 1\%, 5\%, 8\%$ 条件下分别进行了模拟，其中在 $\Phi=5\%$ 时进行了相位角解析。关于模拟中边界条件的设置，通过半步长反弹格式^[22]将搅拌槽上、下表面和槽壁设置为无滑移壁面，并通过浸入边界条件^[13,23,24]对搅拌桨表面和颗粒表面进行无滑移处理。模拟中碰撞过程被分成两类来处理：采用基于双参数(恢复系数、摩擦系数)模型^[25]的硬球碰撞算法来模拟颗粒间以及颗粒和搅拌槽上、下表面及槽壁间的碰撞过程；软球碰撞模型被用来处理颗粒和搅拌桨间的碰撞过程^[4,19]。

2 结果与讨论

本课题组^[4]之前在相同体系下进行了过渡流搅拌槽内颗粒悬浮过程的实验、模拟研究，图S1显示了其部分结果。如图S1所示，实验、模拟结果无论是液相平均速度还是液相湍流动能均吻合得很好，其误

图1 (网络版彩色)搅拌槽和搅拌桨的几何尺寸, 坐标系和研究区域(虚线框)。搅拌桨沿顺时针方向转动, 为下压式结构

Figure 1 (Color online) Geometry of the stirred tank and the impeller, coordinate system and the area of investigation (frame with dotted line). The impeller rotates clockwise to pump down the liquid

差主要出现在峰值区. 且当颗粒体积分数 $\Phi=8\%$ 时, 实验、模拟结果间误差最大, 其液相平均径向、轴向速度最大误差分别为13%和16%(图S1(a), (b)); 在 $z/H=0.2$ 处其液相湍动能最大误差为24%(图S1(d)), 而在 $x/T=0.45$ 处的液相湍动能最大误差仅为8%(图S1(c)), 证明了该数值模拟方法的可靠性. 基于此, 本文将主要从数值模拟的角度对过渡流搅拌槽内颗粒悬浮过程的流体力学特性进行讨论、对比、分析.

本文首先在相位角 $\theta=30^\circ$ 条件下, 对比了搅拌槽内单一液相瞬态流场和固-液两相体系($\Phi=8\%$)的液相瞬态流场. 如图2(a)所示, 流体从桨叶叶端排出, 遇到槽壁后沿壁面向上运动并形成较大的旋涡. 图2(b)是图2(a)中白框区域即桨叶叶端区的局部流场, 本研究中颗粒的斯托克斯数:

$$St \equiv \frac{2}{9} \frac{\rho_s}{\rho} \frac{d_p^2 4N}{\nu} = 4.95, \quad (1)$$

其中, ρ_s 为颗粒密度, ρ 为液体密度, 因此颗粒的存在会阻碍液相流体运动, 从而削弱该区域流场. 除液相瞬态流场间的对比, 也在单一液相体系和固-液两相体系间进行了统计平均流体力学特性的对比. 需要指出的是, 接下来本文中所有平均流体力学特性均是在模拟达到近似稳态后, 通过500个瞬态数据文件计算求得.

图S2对比了搅拌槽内颗粒体积分数 $\Phi=5\%$ 时, 不同相位角条件下的液相平均速度场, 并用 $\bar{u}_\theta, \bar{w}_\theta$ 来表示特定相位角 θ 条件下的液相平均径向速度和平均轴向速度. 如图S2所示, 流体从桨叶排出, 遇到壁面后形成两股流体运动, 其中一股流体沿着壁面向

图2 (网络版彩色)搅拌槽内在相位角 $\theta=30^\circ$ 条件下的瞬态流场对比. (a1), (b1)为单一液相体系; (a2), (b2)为固-液两相体系($\Phi=8\%$). 其中(b1, b2)所显示的流场为(a1, a2)中的白框区域, (b1, b2)的图例位于其顶部

Figure 2 (Color online) Comparisons of instantaneous liquid velocity field in the stirred tank at $\theta=30^\circ$ between the single phase system (left column) and the solid-liquid two phase system with $\Phi=8\%$ (right column). The region of sub-figure (b1, b2) in the stirred tank is marked in sub-figure (a1, a2). The reference vector at top applies to sub-figure (b1, b2)

上流动并最终回到桨叶上端从而形成一个较大的旋涡；另一股则沿着壁面向下流动通过槽底回到桨叶下端形成一个较小的旋涡。图3对比了搅拌槽内在相位角 $\theta=30^\circ$ 时，颗粒分率对液相平均流场的影响。当颗粒体积固含率从0%增加到1%时，搅拌槽内液相平均流场没有明显的变化；当颗粒体积分率增加到5%，8%后，与单一液相体系相比，由于搅拌槽内有较多颗粒存在，在近壁面区和槽底液相平均速度均会衰减，而且随着固含率的增加这种衰减会更明显。

最后，对比了不同条件下液相脉动状况，并用液相湍流动能 k 来表示，其计算公式如下：

$$k = \frac{1}{2} (U_\theta'^2 + V_\theta'^2 + W_\theta'^2), \quad (2)$$

其中， U_θ' ， V_θ' ， W_θ' 分别表示在特定相位角 θ 条件下

液体径向、切向、轴向脉动速度。为方便将来与二维PIV(只能测量径向、轴向两个方向上的液相速度)实验数据进行对比分析，现将模拟中液相切向脉动速度做如下近似处理：

$$V_\theta'^2 = \frac{1}{2} (U_\theta'^2 + W_\theta'^2), \quad (3)$$

进而液相湍流动能可近似为^[26]

$$k \approx \frac{3}{4} (U_\theta'^2 + W_\theta'^2). \quad (4)$$

本文中液相湍流动能值均是在特定相位角条件下计算获得的，因此液相脉动只源自于流体运动而非桨叶周期性运动。图S3对比了颗粒体积分率 $\Phi=5\%$ 时不同相位角条件下的液相湍流动能，结果表明湍流动能峰值均出现在叶端区，但峰值位置会随着相

图3 (网络版彩色)不同颗粒体积分率 $\Phi=0\%$ (a), $\Phi=1\%$ (b), $\Phi=5\%$ (c), $\Phi=8\%$ (d)在相位角 $\theta=30^\circ$ 条件下的无因次化液相平均速度场。模拟中流场真实解析率在 x , z 方向上均为本图所显示的3倍

Figure 3 (Color online) Normalized liquid averaged velocity field for different solids volume fractions: $\Phi=0\%$ (a), $\Phi=1\%$ (b), $\Phi=5\%$ (c), and $\Phi=8\%$ (d) at impeller angle $\theta=30^\circ$. The resolutions of the simulations are three times as high in each direction as the density of the velocity vectors in this figure

位角的改变而移动,当相位角从 0° 增加到 30° 时,峰值位置沿垂直方向明显向下移动;当相位角从 30° 增加到 60° 时,峰值位置沿垂直方向略向上移动.此外,随着相位角的增加,湍流动能峰值也会改变,当相位角从 0° 增加到 30° 时,峰值处湍流动能值增加超过50%;而当相位角从 30° 增加到 60° 时,峰值处湍流动能值无明显变化.图4比较了在相位角 $\theta=30^\circ$ 时不同颗粒体积分率条件下的液相湍流动能值,结果表明随着固含率的增加,液相湍流动能尤其是峰值处衰减显著,这与之前其他研究者^[2,4,9]的研究结果一致.图5定量比较了在相位角 $\theta=30^\circ$ 时液相湍流动能随颗粒体积分率的变化,如图5(a), (b)所示,当固含率从0%增加到8%时,峰值处湍流动能值分别下降了17%和20%.

3 结论

本文采用LB方法模拟了过渡流搅拌槽内在相位角 $\theta=30^\circ$ 时,颗粒体积分率分别为0%, 1%, 5%, 8%条件下的颗粒悬浮过程,并在固含率为5%时对液相流场进行了相位解析分析.模拟中流场被准确解析,因此可以获得颗粒周围、颗粒间的局部瞬态流场,从而实现了在颗粒尺度上研究搅拌槽内颗粒与其周围流场的相互作用.本文主要从液相瞬态流场、液相平均速度场、液相湍流动能三方面对模拟结果进行对比分析,结果表明,颗粒的存在会阻碍液相流场和湍流动能,并且随着固含率的增加这种阻碍现象越明显.本研究成果的数值模拟结果为将来搅拌槽内颗粒悬浮过程的实验研究提供了重要的参考价值.

图4 (网络版彩色)在相位角 $\theta=30^\circ$ 条件下,不同颗粒体积分率 $\Phi=0\%$ (a), $\Phi=1\%$ (b), $\Phi=5\%$ (c), $\Phi=8\%$ (d)的无因次化液相湍流动能云图

Figure 4 (Color online) Normalized turbulent kinetic energy of the liquid for different solids volume fractions: $\Phi=0\%$ (a), $\Phi=1\%$ (b), $\Phi=5\%$ (c), $\Phi=8\%$ (d) at impeller angle $\theta=30^\circ$

图 5 (网络版彩色) 相位角 $\theta=30^\circ$ 条件下不同颗粒体积分数(0%, 1%, 5% 和 8%) 在 $x/T=0.4$ (a) 和 $z/H=0.17$ (b) 处的无因次化液相湍动能点线图
Figure 5 (Color online) Profile of normalized turbulent kinetic energy of the liquid at $x/T=0.4$ (a) and $z/H=0.17$ (b) for different solids volume fractions 0%, 1%, 5% and 8% at impeller angle $\theta=30^\circ$

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补充材料

- 图 S1** 搅拌槽内不同颗粒体积分数(0%, 5% 和 8%)在相位角 $\theta=60^\circ$ 条件下实验、模拟结果对比
- 图 S2** 不同相位角 $\theta=0^\circ, 30^\circ, 60^\circ$ 在颗粒体积分数 $\phi=5\%$ 条件下无因次化液相平均速度场
- 图 S3** 在颗粒体积分数 $\phi=5\%$ 条件下, 不同相位角 $\theta=0^\circ, 30^\circ, 60^\circ$ 无因次化液相湍流动能云图

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Summary for “过渡流搅拌槽内固-液悬浮的直接数值模拟”

Direct numerical simulations of solid-liquid suspension in a transitional stirred tank

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Solid-liquid stirred tanks are very common in industrial process, for example pharmaceutical engineering, water treatment and crystallization. In these operating units, solid-liquid two-phase flows affect the rates of momentum, mass and heat transfer as well as the chemical reactions significantly. The flow regime in most investigations of solid-liquid suspension is either laminar or turbulent, however the transitional regime is also very important especially when scaling up from bench scale to pilot scale. Therefore, it is important to investigate the hydrodynamic characteristics of solid-liquid suspension in a transitional stirred tank. In this work, the lattice Boltzmann method was used to solve the liquid flow field. The uniform, cubic grids were applied with grid spacing Δ and time step Δt representing the lattice units in space and time respectively. The stirred tank is a cubic tank with a flat bottom, whose height and side length of the bottom are both equal to 264Δ . The impeller is a 45° pitched-blade turbine with diameter $D=189.6\Delta$; width of the impeller blade $W=38.4\Delta$ and it operates under the down-pumping configuration. The impeller-based Reynolds number is 1334, which indicates that the flows belong to transitional regime. The particles are all equally sized solid spheres with diameter $d_p=9.6\Delta$. As for the boundary conditions in this work, the half-way bounce-back rule was used to form the no-slip boundary conditions at all tank walls including top, bottom and side walls. The immersed boundary method was applied to impose the no-slip boundary conditions at the particles' surface and the impeller's surface. When it comes to the collisions, a hard-sphere collision algorithm based on the two-parameters model (restitution coefficient and friction coefficient) was adopted to carry out the collisions among the particles as well as the collisions between the particles and the tank walls. The collisions between the particles and the impeller were performed by using a soft-sphere collision model. In addition, the lubrication force was applied to deal with the close-range hydrodynamic interaction between the solid surfaces. This paper mainly did the simulations for different solids volume fractions $\Phi=0\%$, 1% , 5% and 8% at impeller angle $\theta=30^\circ$ and at the same time resolved the impeller angles to 0° , 30° and 60° for solids volume fraction $\Phi=5\%$. In terms of simulated results, at first we compare the instantaneous liquid flow field between the single-phase system and the solid-liquid two-phase system, which shows that the exist of particles clearly hindered the liquid flow field especially in the impeller-discharge region. This paper also compares the averaged hydrodynamic characteristics between the single-phase system and the solid-liquid two-phase system. The results show that the averaged liquid velocity did not change obviously with the rise of solids volume fraction from 0% to 1% , however, when the solids volume fraction rose up to 5% or even higher to 8% , the averaged liquid velocity decreased obviously in the impeller-discharge region as well as the region near the bottom of the stirred tank at impeller angles $\theta=30^\circ$. Finally, the turbulent kinetic energy (TKE) of the liquid is compared qualitatively and quantitatively and it shows that the TKE values decreased significantly with the rise of solids volume fraction at impeller angle $\theta=30^\circ$. The peak TKE values decreased more than 50% with the rise of impeller angle θ from 0° to 30° for solids volume fraction $\Phi=5\%$, however the peak TKE values did not change obviously with the impeller angle θ rising from 30° to 60° .

solid-liquid suspension, transitional flow, stirred tank, resolved-particle, lattice Boltzmann method

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