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CFD analysis of the turbulent flow in baffled shake flasks

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ABSTRACT

In this work, computational fluid dynamics (CFD) technique is used to simulate the complicated unsteady-state turbulent flow field formed in baffled flask. The baffled flask shows advantages both in mass transfer capacity and in shear formation in comparison with unbaffled flasks. Detailed investigations of power consumption, mass transfer and shear rate are carried out in baffled flasks under shaking frequencies ranging from 100 rpm to 250 rpm, and filling volumes from 50 mL to 150 mL. The results show that the specific power input and specific interface area are both greatly influenced by shaking frequency and filling volume. For the positive effect of shaking frequency on both mass transfer coefficient (k_L) and specific interface area (a), the volumetric mass transfer coefficient (k_La) increases greatly with shaking frequency. Results also show that filling volume has no significant effect on k_L but negative effect on specific interface area. Shear force formed in baffled flask shows great dependent on shaking frequency, but it is insensitive to the filling volume. Based on these investigations, correlations linking these parameters are proposed. Finally, cultivations of filamentous fungus conducted in unbaffled and baffled flasks validated the simulating results.

1. Introduction

Shake flasks are widely used in process development and optimization in biotechnology, such as cell culture, media optimization and strain screening. Culture experiments in flasks are low-cost, easy to operate and can be done in parallel with substantial tests [1]. Recently, the application of shaking microreactors in biological process attracts more and more attention [2–5]. Due to the bottleneck in process monitoring and controlling, however, they have not been fully applied in industry. Thus shake flasks are still the most common reactors used in lab as well as in industry [6].

Scale-up from shake flasks to fermenters is a key step for large scale manufacture. But this process is always hampered because of lacking in knowledge of engineering factors of shake flasks, especially baffled flasks, such as mass transfer, hydromechanics and power consumption [7]. A deep insight into engineering factors of shake flasks, especially hydromechanical study, will provide valuable data and criterions for the design and scale-up of bioreactors. While, due to the limit of measuring methods, it is of great difficulty to obtain these parameters. The reported works are limited in mass transfer [8–14] and power consumption [15–19] in unbaffled flasks. Most of the hydraulic performance investigations of shake flasks are carried out by a physical model [20–22], which is simplified and thus cannot reveal the real process.

Despite the potential advantages in mass transfer, mixing and distinctive shear property for high aerobic microorganism and filamentous fungus fermentation, these engineering aspects of baffled flask is always underestimated, mainly due to the complicated flow field formed in it. Galindo et al. [23] have studied, in baffled flask, the effect of hydrodynamic stress on *Trichoderma* fermentation. While, there is no publication comprehensively elaborating the hydrodynamic characteristics of baffled flasks. Peter et al. [24] developed a device to measure the volumetric power consumption and proposed a relatively comprehensive correlation for calculating volumetric power consumption in baffled shake flask. Over the past decade, with increasing maturity of computational fluid dynamics (CFD), numerical investigations of hydromechanical characteristics in bioreactor have attracted more and more attention. CFD techniques have been widely used in the fluid dynamic investigation of bioreactors [25–27], including the unbaffled flasks [1,28], but have not yet been used in baffled flasks.

The aim of this work is to investigate the hydrodynamic characteristics of baffled shake flasks with CFD method. Unbaffled flasks were studied as a contrast. This study mainly focused on turbulence parameters (e.g. turbulent kinetic energy, energy dissipation and volumetric power consumption), mass transfer and shear environment (e.g. shear strain rate and wall shear force). All parameters were obtained through the simulation and some of them were combined with models of mass transfer to estimate the volumetric mass transfer coefficient. Moreover, reported experimental observations

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Nomenclature

a	specific gas–liquid interface area ($\mathrm{m^2\,m^{-3}}$)
A	gas–liquid interface area ($\mathrm{cm^2}$)
b	constant
B	constant
c	oxygen concentration in liquid phase ($\mathrm{mmol\,L^{-1}}$)
c^*	saturation concentration of oxygen in liquid phase ($\mathrm{mmol\,L^{-1}}$)
$C_{\varepsilon 1RNG}$	RNG k–ε turbulence model coefficient
$C_{\varepsilon 2RNG}$	constant
$C_{\mu RNG}$	constant
d	maximum flask diameter (m)
d_0	shaking diameter (m)
D_L	diffusion coefficient of oxygen ($\mathrm{m^2\,s^{-1}}$)
$\mathbf{F}$	surface tension ($\mathrm{N\,m^{-1}}$)
g	acceleration of gravity ($\mathrm{m\,s^{-2}}$)
H	fluid level (mm)
I	turbulence intensity (%)
k	turbulent kinetic energy ($\mathrm{m^2\,s^{-2}}$)
k_L	oxygen mass transfer coefficient ($\mathrm{m\,h^{-1}}$)
k_La	oxygen volumetric mass transfer coefficient ($\mathrm{h^{-1}}$)
$\mathbf{n}$	unit normal vector
N	shaking frequency ($\mathrm{rev\,min^{-1}}$, or rpm)
p	pressure (Pa)
P_k	turbulence production due to viscous forces
P_{kb}	influence of the buoyancy forces
$P_{\varepsilon b}$	influence of the buoyancy forces
P/V	volumetric power consumption ($\mathrm{W\,m^{-3}}$)
r	radius of gyration (m)
SSR	shear strain rate ($\mathrm{s^{-1}}$)
t	the run duration (s)
u	mean velocity ($\mathrm{m\,s^{-1}}$)
u_{max}	maximum linear velocity of flasks ($\mathrm{m\,s^{-1}}$)
$\boldsymbol{v}$	velocity ($\mathrm{m\,s^{-1}}$)
v	kinematic viscosity of the fluid ($\mathrm{m^2\,s^{-1}}$)
V	filling volume (mL)
WSF	wall shear force (Pa)

Greek letters

β_{RNG}	constant
γ	fraction function
ΔL	grid height (m)
Δt	time step (s)
ε	energy dissipating rate ($\mathrm{m^2\,s^{-3}}$)
κ	surface curvature ($\mathrm{m^{-1}}$)
μ	viscosity of the fluid (Pa s)
μ_t	turbulence viscosity (Pa s)
ρ	density ($\mathrm{kg\,m^{-3}}$)
σ	surface tension coefficient ($\mathrm{N\,m^{-1}}$)
σ_k	constant
$\sigma_{\varepsilon RNG}$	constant
ω	angular velocity ($\mathrm{rad\,s^{-1}}$)

were used to compare with the predictions. Simultaneously, correlation between these parameters and operating conditions was evaluated. Finally, cultivation of filamentous fungus was conducted in unbaffled and baffled flasks to validate the simulating results.

2. Materials and methods

2.1. Flask configurations

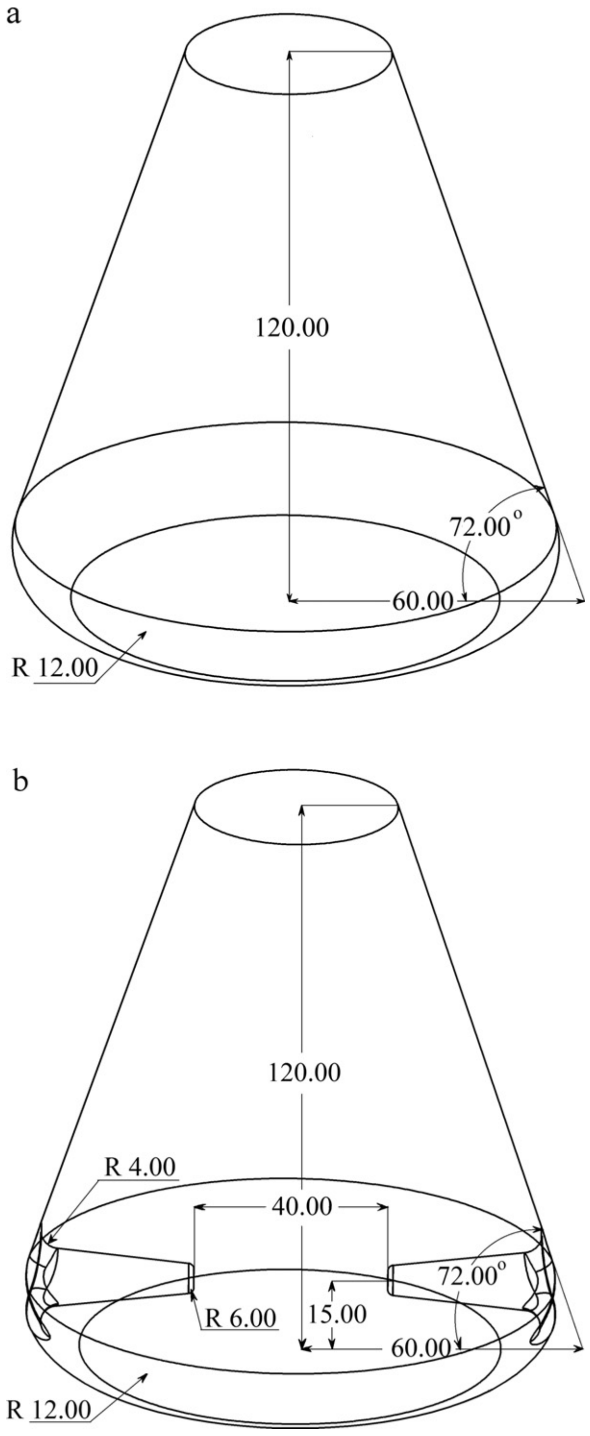

Fig. 1. Geometric dimensions of unbaffled (a) and baffled flask (b).

Flasks used in this study are all 500 mL in capacity. Geometric dimensions are shown in Fig. 1. The baffled flask is symmetrically equipped with two conical baffles at the height of 15 mm. The interval between two baffles is 40 mm. Liquid cannot reach the bottleneck of the flask under operating conditions in this work, so the computational domain only contains the main body of the flask without the neck part.

2.2. Modeling approach

2.2.1. CFD modeling of two-phase flow

There are two phases in the flask, namely, liquid phase at the bottom with gas phase above it. A distinct interface, i.e. the free surface is formed between these two phases. In this study, volume