Modelling of CSTR Flow Field for Agaricus bisporus Residue Fermentation Based on CFD Numerical Simulation

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Modelling of CSTR Flow Field for Agaricus bisporus Residue

Fermentation Based on CFD Numerical Simulation

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Abstract: Agaricus bisporus production gets a lot of residues, which could be fermented by a continuous stirred tank reactor (CSTR). This research was conducted to study the characteristics of the multiphase flow field in the reactor and its influence on the efficiency of biogas production in the CSTR fermentation process of Agaricus bisporus residue by using CFD numerical simulation technique. The aim is to reveal the relationship between the reactor operating conditions, flow field characteristics, and biogas production efficiency at the micro-level. We compared the results of different turbulence models by evaluating the power quotients and flow quotients with the experimental results to derive the most suitable flow field model inside the reactor for the Agaricus bisporus residues. The results showed that, under the condition that the number of grids does not affect the simulation results, and considering the model accuracy and efficiency, the numerical method can be chosen as the multiple reference frame (MRF) method of the second-order upwind discrete scheme with the realizable $k-\varepsilon$ model. In this way, we can make use of edible mushroom residue as a substrate for resource utilization and provide basic data and theoretical basis for the design and scale-up with anaerobic fermentation to biogas reactor.

Keywords: Biogas; Computational fluid dynamics (CFD); Continuous stirred tank reactor (CSTR); Agaricus bisporus residue; Flow field
1. Introduction

Currently, agricultural residues are considered as a recycling resource. Appropriate treatment could make the residues to be energy resources and environmentally friendly (Bentsen et al. 2018). *Agaricus bisporus* residue is a mixture of residual fungus substrates and metabolites after *Agaricus bisporus* harvest (Cengiz et al. 2014). Due to the abundant nutrients in the residue, can be used as raw material for anaerobic fermentation to produce biogas. During anaerobic fermentation, complex polymers are transformed into biogas by methanogenic bacteria (Bedoya et al. 2020). Biogas is one of the most hopeful renewable energy sources nowadays, which has a great benefit both on environmental protection and energy-saving, especially in the treatment of organic waste (Moghtaderi et al. 2006; Gronowska et al. 2009; Kumarappan et al. 2009; Esen & Yuksel 2013). A continuous stirred tank reactor (CSTR) is a widely used bioreactor in biogas engineering, which greatly increases the contact area between microorganisms and fermentation materials owing to the addition of a stirring device compared with other common reactors (Hassan et al. 2020).

In a fermentation reactor, mixing is an important operation to improve the efficiency of biogas anaerobic fermentation and biogas productivity by homogenizing the methanogenic bacteria, nutrients, and temperature throughout the reactor (Moretto et al. 2020; Villamil et al. 2020). Although modern biogas engineering generally incorporates mixing technology to improve fermentation efficiency (Leow et al. 2020), a large number of biogas projects use a simple mixing strategy, which doesn’t help to enhance the efficiency of biogas production, and even consumes more energy (Luan et al. 2014). As the biogas anaerobic fermentation reactor needs to be sealed, it is hard to know the internal flow field of the reactor. So, the added mixing modules probably are not suitable for the reactor shape or the raw material characteristics, resulting in insufficient mixing (Munoz et al. 2018).

Computational fluid dynamics (CFD) modeling can accurately analyze the internal flow state of a biogas anaerobic reactor. It has been widely used in fluid mechanical process optimization to enhance biogas production by improving the mixing structure (Yang et al. 2012; Zou et al. 2012). The mixing process of fermentation fluid is essentially a flow process under the action of external forces, and CFD numerical simulation methods can help people understand its theoretical flow process and flow pattern (Wu 2013). In 2002, North Carolina State University firstly proposed how CFD can be used to investigate the fluid mixing flow patterns of biogas fermentation materials (Fleming & Graham 2002). Since then, many biogas fermentation reactor researchers have made significant progress based on the flow field patterns study. Some researchers have used CFD to visualize and analyze the flow pattern state formed during the mixing process (Mendoza et al. 2011), thus introducing...
methods that can accurately verify and design mixing mechanisms (Ding et al. 2010; Bartzanas et al. 2013). These approaches made the internal mixing conditions in biogas fermentation reactors visualize and quantitative. For example, Luo (Luo et al. 2015) used CFD simulations to find that fermentation efficiency would be better in a long-cylinder anaerobic reactor if the stock was placed from the top and slowly settled by gravity in such a discharge. Marti-Herrero (Marti-Herrero et al. 2014) optimized the mixing flow pattern in the biogas reactor by improving the grid model, which resulted in a 44% increase in biogas production and the smooth operation of the reaction. Dapelo (Dapelo et al. 2015) applied the Euler-Lagrange model to a continuous stirred tank anaerobic fermentation reactor and modeled it using the CFD technique, which was found to be significant for studying the flow field changes inside the reactor. All these studies have shown that the material mixing process can be simulated by the CFD technique, which is an important technical approach to improve the mixing problem inside the reactor. It not only makes the study of mixing conditions inside biogas fermenters largely free from unseen conditions, but also promotes a level of scientific and accurate visualization and quantitative analysis of the research.

The objective of this paper is to study the fluid flow field characteristics on the efficiency of biogas production by CSTR using *Agaricus bisporus* residue as the substrate based on CFD numerical simulation technique. We hope to provide basic data of scale-up and design of anaerobic fermentation biogas reactor used the edible mushroom residue as substrate.

2. Materials and methods

2.1 Reactor geometry

The tank and stirrer structure of the CSTR is shown in Figure 1. The shell of the tank is a traditional and economical circular tank with uniform force distribution. The addition of four vertical baffles can effectively weaken the tangential flow and enhance the axial and radial flow. The mixing mechanism of the reactor was designed as a double-layer paddle combination, with a four four-folded-blade open turbine paddle in the upper layer and a six-straight-blade disk turbine paddle in the lower layer, which was sealed by a shaft seal to the mixing shaft. The fermentation liquid of the *Agaricus bisporus* residue was filled to the hydrostatic level of $H_L=360$ mm, while the effective volume of the reactor was 28L. During mixing, the speed of the stirrer was 60 rpm, which was controlled by an adjustable speed device. There was a circulating water jacket on the outside of the reactor with a temperature control device to make the temperature stable.
2.2 Fluid dynamics governing equations

The fluid flow in CSTR obeys the three conservation laws in fluid mechanics, which satisfied the momentum conservation equation, mass conservation equation, and energy conservation equation.

The mass conservation equation can be expressed as:

\[ \frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \vec{v}) - S_m = 0 \]  

(1)

the above equation refers to the mass of fluid flowing in per unit time is equal to the mass increased to per unit time, in this, \( \rho \) is the fluid density; \( t \) is the fluid flow time; \( \vec{v} \) is the velocity vector; \( S_m \) is the mass source term.

Momentum conservation can be expressed as:

\[ \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u \vec{u}) = -\frac{\partial P}{\partial x} + \nabla \cdot (\mu \nabla u) + S_x \]  

(2)

\[ \frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho u \vec{v}) = -\frac{\partial P}{\partial y} + \nabla \cdot (\mu \nabla v) + S_y \]  

(3)

\[ \frac{\partial (\rho w)}{\partial t} + \nabla \cdot (\rho u \vec{w}) = -\frac{\partial P}{\partial z} + \nabla \cdot (\mu \nabla w) + S_z \]  

(4)

the change rate of momentum per unit time for the fluid is equal to the sum with volume force per unit volume in space, in equation, \( P \) is the pressure exerted on the micro-element body; \( u, v, w \) is the component of the three-dimensional velocity in the three directions; \( S_x, S_y, S_z \) is the volume force applied in the three directions.

The energy conservation equation can be expressed as:

\[ \frac{\partial (\rho T)}{\partial t} + \nabla \cdot (\rho u \vec{T}) = \nabla \left( \frac{k}{c_p} \nabla T \right) + S_T \]  

(5)

assuming that the external force is only the volume force and area force, the change rate of kinetic energy and internal energy of the substance in the region \( \Omega \) is equal to the work done by the volume force and area force per unit time plus the heat given to the substance by the outside world per unit time, in the equation above, \( T \) is the temperature, \( c_p \) is the specific heat capacity, \( k \) is the heat transfer coefficient, \( S_T \) is the heat source of the fluid including the system itself and the energy converted from external energy.

In addition, the rheological equation is an equation that describes the relationship between fluid shear stress and fluid gradient for the mechanics to which the substance is subjected, of which the power law model is most commonly used and can be expressed as:

\[ \eta = K \gamma^{n-1} \]  

(6)
where $\eta$ is viscosity, $K$ is the consistency coefficient, $\dot{\gamma}$ is the shear rate, $n$ is the power law exponent.

This study mainly focused on the isothermal simulation of the internal flow of CSTR, and the heat transfer is not involved, so the law of energy conservation is not repeated.

### 2.3 Definition of dimensionless number

Since the fermentation fluid of *Agaricus bisporus* residue was an isothermal incompressible fluid at the fermentation temperature at 323.15 K and exhibits a non-Newtonian pseudo-plastic fluid behavior. Therefore, in the mechanically stirred reactor, the Reynolds number (Re) of the non-Newtonian fluid is expressed as (Chen 1981):

$$Re = \frac{\rho N D^2}{\eta} \quad (7)$$

where $N$ is the rotating speed of the impeller, $D$ is the diameter of the impeller, and $\eta$ is determined by equation (6) in which the shear rate can be indicated as:

$$\dot{\gamma} = K_S N \quad (8)$$

where $K_S$ is a constant determined experimentally.

In a similar way to pipe flow, the Reynolds number of a fluid flowing through a moving zone can be expressed as:

$$Re_g = \frac{\rho U_\infty D^n d^n}{K(0.75 + \frac{21}{n}) n g^{n-1}} \quad (9)$$

where $U_\infty$ is the average velocity of the fluid at the exit of the moving zone, and $d$ is the diameter of the moving zone.

The power quotient ($N_P$) and the flow quotient ($N_Q$) in the mixing vessel are expressed as (Paul et al. 2004):

$$N_P = \frac{P}{\rho N^3 D^5} \quad (10)$$

$$N_Q = \frac{Q}{N D^5} \quad (11)$$

where $P$ is the power input, and $Q$ is the flow rate through the moving zone.

### 2.4 Mathematical models and solution methods

The CFD preprocessing software GAMBIT and the commercial CFD package Fluent 2020R1 (ANSYS-Fluent, Inc., 2020) were used in this study. CFD modeling includes preprocessing, model setup, iterative
calculations, and post-processing of the results. Both the baffle and impeller blades were treated as zero-thickness walls in the preprocessing to reduce the number of meshes. The multiple reference frame (MRF) was used in this study to deal with the rotation in the stirrer region. MRF is a steady-state approximation method but gives good simulation results in non-steady-state problems. The whole CSTR computational domain is decomposed into several subdomains, i.e., rotational domain and stationary domain with different reference systems set for each subdomain in the MRF. The shaft and the paddle of the stirrer were moving boundaries, and when the stirrer was in the rotational domain, the motion has the same speed as the fluid in this subdomain; when the stirrer was in the stationary domain, it was moving compared to the fluid in this subdomain. The stirrer subdomain in the reactor adopted the non-inertial coordinate system with synchronous rotation to the stirring shaft, while the inertial coordinate system was used in the stationary domain of the reactor besides the stirrer.

### 2.5 Boundary conditions and initial conditions

In this study, the flow field was numerically simulated for the fermentation fluid of *Agaricus bisporus* residue in CSTR, where the material was characterized as a gas-liquid-solid three-phase fluid with small solid particles. Some research (Hooshyar et al. 2013) results showed that when the solid phase particle diameter at 0.078-0.587mm, there was no collision effect between solid particles and bubbles, and they followed the main fluid movement; when the particle diameter was 2.0-4.0mm, the particles were not easily followed by the liquid phase flow, the solid phase and gas phase had obvious collision occurring at this time, which would make the bubbles occurred deformation effect and impact the movement speed of bubbles. Due to the *Agaricus bisporus* residue after being crushed and sieved, the obtained particles were less than 0.5 mm. According to the above study, the effect between particles and bubbles can be ignored, therefore it can be considered as a gas-liquid two-phase system.

With the selection of double-precision and the 3D model in Fluent software, the boundary conditions and initial conditions were set as follows:

1. Selected the pressure-based solver, and the time was set to transient mode, and the gravitational acceleration in Z direction was set to \(-9.81 \text{m/s}^2\).

2. Since the medium in CSTR was biogas and *Agaricus bisporus* residue fermentation broth, the multiphase flow model was adopted as methane and water, where the density and viscosity of water were changed to the value of *Agaricus bisporus* residue fermentation broth to simulate its slurry phase. The multiphase flow
models in Fluent are powerful in the calculation, including the volume of fluid (VOF) model, the mixture model
and the Eulerian model, and different multiphase flow models are used for different flow forms. Therefore, it is
necessary to choose a suitable multiphase flow model for the material characteristics of this study, and because we
mainly investigated the flow field distribution patterns of gas-liquid two phases, the Eulerian model was finally
chosen.

3. The fluid flow in bioreactor mainly includes laminar flow and turbulent flow, in which turbulence is
more common and its flow is more complicated. When using CFD to deal with turbulence problems, an appropriate
model is crucial to characterize the flow field (Wu 2011). Turbulence models are generally classified into three
types: Reynolds-averaged Navier-Stokes (RANS) models, large eddy simulation (LES) models, and direct
numerical simulation (DNS) models. Among them, the RANS model is less computationally intensive and can
simulate basically all fluid turbulent motions. For this feature, this study mainly focused on the subordinate model
in the RANS turbulence model for simulation analysis.

The RANS model, which averages the transient turbulent flow in time by using the Navier-Stokes
equation, is characterized by its less amount of computation and its ability to simulate almost all fluid turbulent
motions. The RANS model contains a series of affiliated models: such as the k-epsilon model, the k-omega model,
the Reynolds-Stress model, etc. Compared with the RANS model, the LES model is only used for larger-scale
vortices by filtering functions, which require more computation meshes and computational amount. Without
making any turbulence assumptions and solving the transient Navier-Stokes equation directly, the DNS model has
the advantage that all turbulence characteristics can be calculated but cost much. Therefore, in comparison, the
most economical and efficient turbulence model is RANS for this study.

The turbulence model in this study was based on the RANS model, which included one-equation \( k \),
two-equation \( k - \epsilon \) or \( k - \omega \), the RSM, etc. Some researchers used a low-Reynolds-number \( k - \epsilon \) model to
simulate the anaerobic digestion mixing process, and it was found that the computational cost is high even though
it is superior to the other two-equation models (Wu 2010). Meanwhile, the researchers pointed out that the standard
\( k - \omega \) and realizable \( k - \epsilon \) models can be used as recommendations in mechanical mixing of non-Newtonian
fluids (Wu 2011). The fluid in the CSTR was powered by the stirrer and its flow was turbulent. Since the stirrer
rotates faster than the slight rotation, the standard \( k - \omega \) model with shear flow correction, the realizable \( k - \epsilon \)
model and the RSM (Reynold stress model) were used in this study for computational simulation to compare the
applicability of the three models. Table 1 shows the general scope of application and advantages of the three RANS
models.
4. The boundary conditions were set to pressure inlet, only the gas entry was considered, the volume fraction of methane was set to 1, the top outlet allowed only the gas phase to flow out, and the side outlet was set as the wall. The reactor shell, stirrer, and shaft were also set as the wall, and the rotational coordinates and rotational speed of the stirrer and shaft were set separately to distinguish the relative and absolute velocities between them.

3. Results and discussion

In a mixing and stirring reactor, the power number of the impeller is similar to the friction coefficient in a pipe flow, or the drag coefficient of a solid object immersed in the flow. While the power number is inversely proportional to the Reynolds number when the fluid is in laminar flow, it is constant and independent of the Reynolds number in a turbulent flow. The turbulence model tests in this study were conducted in an elliptical bottom cylindrical reactor as shown in Figure 1, with four uniformly distributed baffles and a double layer stirrer arranged inside. The mixing unit consisted of a four-folded-blade open turbine paddle and a six-straight-blade disk turbine paddle, as shown in Figure 2. And the fluid inside the reactor is a non-Newtonian fluid, then in the experiment, the power quotient and flow quotient of the impeller were 0.77 and 0.39 respectively. To quantitatively evaluate the performance of the turbulence model, three error indicators were proposed:

\[ \delta_P = \left| \frac{N_{P,P} - N_{P,lab}}{N_{P,lab}} \right| \times 100\% \]  

\[ \delta_Q = \left| \frac{N_{Q,Q} - N_{Q,lab}}{N_{Q,lab}} \right| \times 100\% \]  

\[ \delta = 0.5(\delta_P + \delta_Q) \]

where \( \delta_P \) and \( \delta_Q \) are errors for predicted power and flow numbers, \( N_{P,lab} \) and \( N_{Q,lab} \) are obtained from the lab specifications, and \( \delta \) is the weighted mean error.

3.1 Grid model assessment

The quantity and quality of the mesh directly affect the accuracy of the computational results. When the mesh quantity is too small, the model cannot have a reasonable mesh assignment, which makes the whole mesh quality low, so the computational accuracy is seriously reduced, and the computation will not be carried out smoothly. And when the number of meshes is too large, it will require higher computer configuration, making the
computational time longer and reducing the work efficiency significantly. To determine the effect of mesh quantity on the simulation results in the CSTR, this study used six sets of meshes for computations with the mesh division numbers of 248936, 485423, 603584, 875067, 1248962, and 1756961. In addition, the turbulent kinetic energy and turbulence intensity of the six mesh models were compared as shown in Figure 3.

Fig 3.

The figure illustrates the variation of turbulent kinetic energy as well as turbulent intensity with the change of mesh number. When the mesh number is from 240,000 to 870,000, the turbulent kinetic energy and turbulent intensity decrease sharply; and then they are level off gradually when the mesh number is from 880,000 to 1,800,000. So, it can be seen that the influence on the numerical analysis results is not obvious when the mesh number is more than 800,000. Considering the mesh quality, computational accuracy, computational volume, and computer configuration requirements, this study selected the mesh number of 875067 for the CFD simulation of CSTR.

In order to further assess the independence of the meshes, the numerical simulation results were compared with 603584, 875067, and 1248962 grid numbers respectively. Due to the symmetry of the constructed CSTR model, the velocity distribution on this cross-section during the stirring paddle operation also has symmetrical characteristics. In this study, we took the cross-section 180 mm above the origin of the CSTR model and compared the velocity variation on this cross-section, and used the velocity of this cross-section on the radius of the X-Y plane as the object of analysis, as shown in Figure 4.

Fig 4.

From Fig. 4, it can be seen that the maximum relative error between mesh numbers 875067 and 1248962 is 3.33%, which is smaller than the maximum relative error between mesh numbers 603584 and 875067, which is 8.54%, so we concluded that continuing to increase the number of meshes would no longer improve the computational accuracy significantly, and the mesh size can already reach the computational accuracy requirement. Furthermore, using a large number of meshes does not improve the prediction of the model because it produces a high discretization error. Therefore, the CSTR model with a mesh number of 875067 was adopted for further simulation.

3.2 Evaluation of turbulence models

Considering that the Agaricus bisporus residue exhibits incompressible non-Newtonian fluid properties
when the temperature is 323.15 K and the inoculum concentration is 50%, and the rheological properties are similar
to water, the Reynolds number can be determined by equations (7) and (8) when the impeller speed \( N = 60 \text{ rpm} \),
which yields \( Re = 3710 \), and Table 2 shows the Reynolds number values under different turbulent flow models.
Based on the input of these parameters, three turbulence models were used for the numerical simulation of the
\textit{Agaricus bisporus} residue fluid within the CSTR. Table 3 shows the power quotients and flow quotients predicted
by equations (10) and (11), where the torque and pumping capacity of each simulated impeller were obtained by
post-processing. The results illustrate that the performance is better in predicting the flow quotients than the power
quotients in CFD numerical simulations, and the realizable \( k - \varepsilon \) model can be realized with the highest accuracy
in the prediction results of the power quotient and flow quotient, and the standard \( k - \omega \) model has higher
accuracy in the prediction of the power quotient than the RSM model, while the prediction accuracy of the flow
quotient is lower than that of the RSM model.

Table 2.

Table 3.

Table 3 also shows the weighted mean error values in the three turbulence models, where equal weights
are assumed for the power quotient and the flow quotient. If the errors are generated during numerical
computations and experiments, this turbulence model can be considered as having excellent prediction results
when \( \delta \leq 10\% \). However, because there is no quantitative criterion for evaluating the turbulence model, and
considering the efficiency of the calculation as well as the economy, we can set the error standard value \( \delta \leq 30\% \),
the prediction results of the turbulence model are applicable. Combining the error analysis and the convergence
results of each run, we found that all three turbulence models were able to predict the mechanical stirring of the
\textit{Agaricus bisporus} residue fluid within the CSTR at an operating condition of 323.15 K, with appropriate CPU
operation time and high stability. Among them, the realizable \( k - \varepsilon \) model performs slightly better than the other
two models, the standard \( k - \omega \) model converges relatively fast, and the RSM has the highest computational cost.
Consequently, in the flow of mechanical stirring, it is recommendable to use the realizable \( k - \varepsilon \) model and
switch to the RSM if needed.

3.3 Changes in the flow pattern of the fluid field

When simulating the flow pattern of a flow field, in general, based on the empirical value of \( K_s \), the
Reynolds number of a non-Newtonian fluid during mechanical stirring can be calculated by equations (7) and (8)
to determine the flow regime (laminar, transition or turbulent). For some commonly used impellers, the experimental data of $K_s$ have been much studied. However, if $K_s$ is unknown for the impeller, the flow information of the moving zone can be used to calculate the Reynolds number ($Re_g$) defined by equation (9). As Table 2 shows the $Re$ and $Re_g$ values in different turbulence model calculations, it can be seen that the differences are not significant. Therefore, when the $K_s$ is unknown, the $Re_g$ value calculated from the moving zone is an acceptable value within the error range. In this study, as $K_s$ was unknown, the simulation analysis was based on using $Re_g$ values.

After obtaining the converged flow field, the flow pattern within the CSTR can be visualized. Take N=60 rpm as an example, Figure 5 shows the global velocity vector diagram in the vertical plane in the middle of the four baffles, which is the flow field characteristic of the two impellers during anaerobic fermentation. When the impellers start to rotate, due to the double-layer paddles of the reactor, the impeller blades drove the fermentation broth downward to the bottom of the vessel. Meanwhile, the fermentation broth flow radially toward the sidewalls of the reactor when it has undergone radial diffusion and separately flow upward and downward along the walls. So, the fermentation broth would form a larger circulation near the upper four-fold blades and two smaller circulations near the lower six-straight-blade disk turbine paddle before returning axially to the upper part of the double-layer impeller. As shown in figure 5, the contour bars represent the velocity scale from zero (blue area) to the maximum value (red area), where the velocity amplitude is greater than (or equal to) the specified maximum value. This method was applied to all the visualized flow field contour plots in this study.

**3.4 Impact of discrete schemes**

For the partial derivative equations established in the solution domain, there are theoretically exact solutions, but due to the complexity of the fluid flow problems dealt with, it is generally difficult to obtain exact solutions to the equations. Therefore, it is necessary to treat the dependent variables at a finite number of locations (grid nodes or grid centroids) in the computational domain as fundamental unknowns by numerical methods, so as to build a set of algebraic equations about these location quantities, and then obtain these node values by solving the set of algebraic equations, while the values at other locations in the computational domain are determined according to the values at the node locations. In this way is how the discrete equations were established, while the discrete scheme is also called interpolation method, as shown in Table 4 for the discrete scheme types utilized in
To investigate the effect of the discrete equations on the power quotients and flow quotients, the momentum equation was set to the second-order upwind differential discrete equation, and the other settings were kept constant. To save computational time, the iterations started from the first-order upwind differencing discrete equation, and then switched to the second-order discrete equation. Numerical simulations were performed for the three types of turbulence models separately, as the results in Table 5 show that the power quotient of the standard $k - \omega$ model decreases from 0.67 to 0.66, with a 1.3% increase in its error value, while the flow quotient improves significantly, from 0.32 to 0.36, with a 10.3% decrease in its error value. For the realizable $k - \varepsilon$ model, the power quotient drops from 0.70 to 0.69 and its error value increases by 1.3%, and the flow quotient raises from 0.37 to 0.38, and its error value reduces by 2.5%. Besides, the power quotient of the RSM model decreases from 0.65 to 0.63 and its error value increases by 2.6%, but the flow quotient increases from 0.35 to 0.37, and its error value decreases by 5.2%. In summary, the simulation analysis using the second-order upwind discrete format has improved the accuracy of its predicted flow quotients, however, the accuracy of the power quotients has decreased. Consequently, if the flow collimator is the main parameter of interest, the second-order upwind differencing discrete equation can be used.

### 3.5 Impact of numerical methods

When the stirring mechanism in a reactor rotates, fluid separation with vortex generation occurs behind its impeller, and the vortex is transmitted to the flow body through convective and turbulent flow, and the flow field motion appears periodic. As a result, a key issue in the CFD numerical simulation of stirred reactors is the simulation of impeller rotation and the resolution of the interaction between the moving impeller and the stationary baffle. The commonly used numerical simulation methods are the impeller boundary condition method, the momentum source-sink method, the inner-outer iterative procedure method, the multiple reference frame (MRF) method, and the sliding-grid method, as shown in Table 6 for the definition of the two numerical methods used in this study their characteristics.
In this study, to investigate the effect of numerical methods on the power and flow quotients, simulations were built based on the convergence of the flow field by the MRF method and then by the Sliding-grid method. This modeling strategy requires switching the conformal interface between the moving and stationary regions to a non-conformal interface. As the Sliding-grid method solves the transient flow field problem, the grid around the stirred impeller is physically shifted during the solution process. Typically, the impeller torque versus time shows a sinusoidal curve with a periodicity, where the highest value occurs at the moment when the blade tip reaches the baffle, and the lowest value occurs when the blade tip reaches the midpoint of the two baffles. The torque on the highest value was taken to calculate the power quotient, as the four-blade tips were set to face the four baffles in the pre-processing of Gambit. Table 7 shows the power quotients and flow quotients predicted by the Sliding-grid method with the grid model setting unchanged. Combing with Table 3 for the MRF method, it can be seen that the \( N_P \) value of the standard \( k - \omega \) model rises from 0.67 to 0.69, with a \( \delta_P \) reduction of 2.6%, and the \( N_Q \) value rises from 0.32 to 0.34, with a \( \delta_Q \) reduction of 5.2%. The \( N_P \) value obtained from the realizable \( k - \epsilon \) model increases from 0.70 to 0.73, with \( \delta_P \) decreasing by 3.9%, and the \( N_Q \) value remains unchanged. The RSM model predicted the \( N_P \) value to increase from 0.65 to 0.67 with a 2.6% decrease in its \( \delta_P \), while there is no change in the \( N_Q \) value. The summary of the above, compared with the MRF method, the Sliding-grid method improves the prediction results overall, but it requires longer CPU time to obtain a solution. From an engineering point of view, the MRF method is recommended because its accuracy is within the acceptable range and its computational cost is low.

### 3.6 Model Validation

Model validation was carried out in the laboratory of the Department of Agricultural Engineering, Fujian Agriculture and Forestry University. During the experiment, 25% inoculum concentration of *Agaricus bisporus* residue was mechanically stirred in a CSTR with an elliptical-bottomed cylindrical reactor shape with four internal baffles, equipped with a four-folded-blade open turbine paddle and a six-straight-blade disk turbine paddle (D=86 mm). The fermentation temperature was maintained at 323.15 K and the impeller was operated in N=60 rpm mode measured by a sensor. Due to the uniqueness of the two-paddle structure and the rheological properties of the *Agaricus bisporus* residue, the CFD numerical simulations were simplified for the reactor and simulated *Agaricus bisporus* residue properties similar to water. Figure 6 shows the comparison of simulated and measured axial velocities with the radial position at z = 180 mm. The CFD predictions are in reasonable agreement with the
measurements when impeller replacement, the use of rheological property approximations, measurement inaccuracies, and numerical errors are taken into account. It shows that the prediction results of realizable $k-\varepsilon$ model among the three types of models is closer to the experimental values. In addition, when using the grid number of 875067, the discretization scheme of first-order upwind format, and the numerical simulation method of MRF method, the weighted average errors are within 30% of both of the power quotients and flow quotients of the predicted models (Table 8), indicating that the simulation results are acceptable.

Fig 6.

Tab 8.

4. CFD visualization of the impeller blade

4.1 Velocity cloud plot of longitudinal section distribution

The velocity cloud plot is used to represent the different velocities in different colors after the CFD simulation calculation, so it can visually describe the velocity distribution in each region of the reactor. Since the baffles can change the fluid flow pattern developed by the stirring paddles, the plane directly perpendicular between two baffles was selected as the cutting surface for observation. Figure 7 shows the velocity distribution cloud in the longitudinal section, it can be seen that the maximum velocity of each paddle is located at the end of each paddle, and it can be clearly observed that the fluid velocity in the rotation region of each paddle decreases in a gradient from the paddle area to the wall direction.

Fig 7.

There is a velocity dead zone below the lower six-straight-blade disk turbine paddle, where the mixing and transfer of material take place mainly by free diffusion. The formation of the bottom stirring dead zone may be the result of flow field circulation and gas-liquid two-phase interaction. It also can be seen that the bottom of the reactor has some radial flow, the disturbance from the stirring paddles develops below the top surface of the upper paddles rather than throughout the reactor. This not only has no influence on the adequate mixing of fluids in the paddling zone, but also provide a stable flow field environment for microbial growth and metabolism.

4.2 Velocity cloud plot of cross section distribution

The impeller blades are the power source of all fluid flow in the reactor, and the fluid flow in the impeller
zone largely determines the mixing of the fermentation broth in the whole reactor. Therefore, studying the velocity
distribution of the fluid in the paddling zone helps us to have a comprehensive understanding of the role of the
stirring paddle. In this paper, the cross-section of the paddles was selected as the object of study, and the center
planes of the upper and lower paddles were analyzed separately to obtain the visualization cloud diagram of the
stirring paddle combination as shown in Figure 8. The figure shows that the liquid near the baffle became turbulent
due to the action of the baffle, and a small vortex appears behind the baffle, which effectively prevents the
formation of large vortices throughout the reactor.

Fig 8.

The tangential flow generated by the rotation is transformed into radial and axial flow by the baffle, which
increases the shear strength of the fluid and thus improves the mixing efficiency. In this way, the baffle can improve
the circulation of the main body, increase the mixing efficiency in the reactor, and make the stirring result more
desirable. In addition, we can clearly observe from it that the peak velocity is distributed in the paddle end region
and spread around the reactor. An axial motion is generated near the four-folded-blade open turbine paddle, and
the blade inclination lead to an oblique upward motion of the paddle wake, which folds when it hits the reactor
wall and the reactor bottom, forming an axial circulation loop, and the paddle action cannot reach the top of the
mixing tank, and these findings are consistent with the velocity vector plot observations. In the lower six-
bladed disk turbine paddle velocity cloud diagram, it can be seen that the flow field perturbation are more intense
and the perturbation spreads outward from the tip of the stirring paddle and folds back after hitting the inner wall
of the reactor, thus forming a complete circulation.

5. Conclusion

By comparing the power quotients and flow quotients of the three types of turbulence models under
different conditions, it is found that the realizable \( k - \varepsilon \) model has the best performance. When a non-Newtonian
fluid moves in a stirring machine, the value of \( K_s \) is an agnostic quantity, then the flow state can be judged by the
Reynolds number calculated from the moving region and then conservatively valued. In choosing the discretization
scheme, when the momentum conservation equation was set to the second-order upwind discretization, the
predicted flow quotients were more accurate, but the accuracy of the power quotients decreased. Among the effects
of numerical methods on model results, the comparison of predicted and experimental values showed that the
Sliding-grid method was more accurate than the MRF method in predicting power quotients and flow quotients,
but with the consideration of computationally intensive and computation time, it is more efficient to use the MRF method in practice. In summary, in the anaerobic fermentation CSTR of *Agaricus bisporus* residues, the standard $k - \omega$ model with a first-order upwind discretization scheme and MRF method can be used when the accuracy demand is low, and the computation time is required to be fast. When a certain accuracy is guaranteed and the calculation time is appropriate, the second-order upwind discretization format with MRF numerical method can be altered as the realizable $k - \varepsilon$ model. The RSM model with a combination of the second-order upwind discretization format and the Sliding-grid method can be used when the accuracy requirement is higher.
Appendix:

Tab 1. Advantages and disadvantages of three RANS models and applications.

<table>
<thead>
<tr>
<th>Model Category</th>
<th>Features and application occasions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Realizable k-epsilon</td>
<td>Suitable for complex shear flows involving rapid strain, slight rotation, vortices, and local transition flows (e.g., delimited layer separation, large-scale separation, and obtuse body wake vortex shedding, large-angle diffuser stall, indoor ventilation, etc.).</td>
</tr>
<tr>
<td>RNG k-epsilon</td>
<td>Most of the advantages are similar to Realizable k-epsilon but harder to converge than it. Suitable for strong rotation cases (e.g., rotating machinery).</td>
</tr>
<tr>
<td>RSM</td>
<td>The most physically sound RANS model with the isotropic vortex viscosity assumption was removed. Higher requirements for computer CPU and the high coupling strength between equations, thus more difficult to converge. Suitable for complex 3D flows involving strong streamline curvature and strong rotation (e.g., curved pipes, rotating flow channels, rotating combustors, cyclones, etc.).</td>
</tr>
</tbody>
</table>

Tab 2. Reynolds number for different turbulence models.

<table>
<thead>
<tr>
<th>Turbulence model types</th>
<th>Reg</th>
<th>Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard k-ω</td>
<td>3867</td>
<td>4.2</td>
</tr>
<tr>
<td>Realizable k-ε</td>
<td>3740</td>
<td>0.8</td>
</tr>
<tr>
<td>RSM</td>
<td>3525</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Note: Temperature=323.15 K; Inoculum Concentration=50%; N=60 rpm; Re=3710.

The error calculations were based on the Reynolds number obtained from equation (7).

Tab 3. Power quotients and flow quotients for different turbulence models.

<table>
<thead>
<tr>
<th>Turbulence model types</th>
<th>$N_p$</th>
<th>$\delta_p$ [%]</th>
<th>$N_q$</th>
<th>$\delta_q$ [%]</th>
<th>$\delta$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard k-ω</td>
<td>0.67</td>
<td>13.0</td>
<td>0.32</td>
<td>18.0</td>
<td>15.5</td>
</tr>
<tr>
<td>Realizable k-ε</td>
<td>0.70</td>
<td>9.1</td>
<td>0.37</td>
<td>5.1</td>
<td>7.1</td>
</tr>
<tr>
<td>RSM</td>
<td>0.65</td>
<td>15.6</td>
<td>0.35</td>
<td>10.3</td>
<td>13.0</td>
</tr>
</tbody>
</table>

Tab 4. The discrete scheme types utilized in this study.
Discrete scheme type | Definitions and characteristics
--- | ---
First-order upwind scheme | It means that the unknown quantity on the interface takes the value of the upstream node constantly. It does not cause any oscillation of the solution under any calculation conditions and is stable. However, when \( Pe \) is large, the pseudo-diffusion is serious, and it is often necessary to encrypt the grid.
Second-order upwind scheme | The second-order upwind format is similar to the first-order upwind format in that both determine the physical quantities controlling the volume interface from the physical quantities of the upstream cell nodes. However, the second-order format uses not only the value of the nearest upstream node but also the value of another upstream node.

Note: \( Pe \) represents the ratio of ‘convection/diffusion’ intensity.

Tab 5. Power quotients and flow quotients under the influence of discrete schemes.

<table>
<thead>
<tr>
<th>Turbulence model types</th>
<th>( N_p )</th>
<th>( \delta_p [%] )</th>
<th>( N_q )</th>
<th>( \delta_q [%] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard k-( \omega )</td>
<td>0.66</td>
<td>14.3</td>
<td>0.36</td>
<td>7.7</td>
</tr>
<tr>
<td>Realizable k-( \varepsilon )</td>
<td>0.69</td>
<td>10.4</td>
<td>0.38</td>
<td>2.6</td>
</tr>
<tr>
<td>RSM</td>
<td>0.63</td>
<td>18.2</td>
<td>0.37</td>
<td>5.1</td>
</tr>
</tbody>
</table>

Tab 6. Definition and characteristics of the numerical simulation methods used in this study.

<table>
<thead>
<tr>
<th>Numerical simulation methods</th>
<th>Definition and Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiple Reference Frame (MRF)</td>
<td>This is a steady-state calculation method in which the rotational coordinates are used as the reference system in the cylindrical stirring region, while the fixed coordinates are used as the reference system in the rest of the region, and the coupling of the rotational coordinate system region with the fixed coordinate system region is done through the boundary conditions of various physical scalars. The advantage is that the overall numerical simulation of the flow field in the stirred reactor is achieved, and experimental assistance is no longer required.</td>
</tr>
</tbody>
</table>
Sliding-grid Method

This is a non-stationary calculation method, which is suitable for the prediction of the strong interaction regime of paddles and baffles, as well as for the study of some transient flow details of the start-up or periodic processes. The biggest drawback of this method is that the calculation requires a lot of time and a more complicated post-processing process.

Tab 7. Power quotient and flow quotient after changing the numerical simulation method.

<table>
<thead>
<tr>
<th>Turbulence model types</th>
<th>( N_P )</th>
<th>( \delta_P % )</th>
<th>( N_Q )</th>
<th>( \delta_Q % )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard k-( \omega )</td>
<td>0.69</td>
<td>10.4</td>
<td>0.34</td>
<td>12.8</td>
</tr>
<tr>
<td>Realizable k-( \varepsilon )</td>
<td>0.73</td>
<td>5.2</td>
<td>0.37</td>
<td>5.1</td>
</tr>
<tr>
<td>RSM</td>
<td>0.67</td>
<td>13.0</td>
<td>0.35</td>
<td>10.3</td>
</tr>
</tbody>
</table>

Tab 8. Weighted mean error values for different model schemes.

<table>
<thead>
<tr>
<th>Turbulence model types</th>
<th>First-order upwind method + MRF method</th>
<th>Second-order upwind method + MRF method</th>
<th>First-order upwind method + Sliding-grid method</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta [%] )</td>
<td>( \delta [%] )</td>
<td>( \delta [%] )</td>
<td></td>
</tr>
<tr>
<td>Standard k-( \omega )</td>
<td>15.5</td>
<td>11.0</td>
<td>11.6</td>
</tr>
<tr>
<td>Realizable k-( \varepsilon )</td>
<td>7.1</td>
<td>6.5</td>
<td>5.2</td>
</tr>
<tr>
<td>RSM</td>
<td>13.0</td>
<td>11.7</td>
<td>11.7</td>
</tr>
</tbody>
</table>
Fig 1. The geometry of the reactor for biogas production from Agaricus bisporus residue with dimensions in mm. The reactor was equipped with 2 turbine paddles and 4 baffles. During anaerobic fermentation, the reactor has a liquid static height of 360mm.

Fig 2. Two impellers for CFD simulation. Note: (a): the four-folded-blade open turbine paddle; (b): the six-straight-blade disk turbine paddle.

Fig 3. Variation curves of turbulent kinetic energy and turbulent intensity for different grid numbers.
Fig 4. Variation curve of velocity with distance for different grid numbers.

Fig 5. Global velocity vectors in the vertical plane inside the reactor.

Fig 6. Comparison of CFD simulation results of axial velocity in different turbulence models with experimental values.
Note: Where a positive value means the velocity direction is vertically upward along the axis and a negative value means the velocity direction is vertically downward along the axis.

**Fig 7.** CSTR internal longitudinal section velocity distribution cloud diagram.

**Fig 8.** Cloud diagram of velocity distribution in the center cross-section of two layers of paddles.
Note: (a) represents the upper four-folded-blade open turbine paddle; (b) represents the lower six-straight-blade disk turbine paddle.
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Contributions:
Xuan Wei formulated the research questions and identified the research ideas. Jinping Zou provides test material. Jiayu Li completed the theoretical and empirical analysis, and was a major contributor in writing the manuscript. All authors read and approved the final manuscript.

Corresponding author:
Xuan Wei.

Ethical Declarations

Competing interests: The authors declare that they have no conflict of interest.

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Consent to Participate: Not applicable.

Consent to Publish: Not applicable.

Availability of data and materials: The datasets used or analyzed during the current study are available from the corresponding author on reasonable request.
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