AND TECHNOLOGY

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# Computational Fluid Dynamics Modeling of Fermentation Reactions in Bioethanol Fermentor: A Review



Ali Satria Wijaya<sup>1\*</sup>, Novia Novia<sup>2\*</sup>, Fitri Hadiah<sup>2</sup>

<sup>1</sup>Post Graduate Program (Master Candidate), Sriwijaya University, Palembang, Indonesia

<sup>2</sup>Departement of Chemical Engineering, Faculty of Engineering, Universitas Sriwijaya, Jl. Raya Palembang-Prabumulih KM 32 Inderalaya Ogan Ilir (OI), Sumatera Selatan, 30662, Indonesia

ABSTRACT: Bioethanol is a renewable energy source that can replace fossil fuels. The advantages in terms of economy and its impact on the environment make bioethanol was chosen as a biofuel. Bioethanol can be produced from various types of biomasses with the help of microorganisms, namely yeast, for the fermentation process. In manufacturing, factors including temperature, concentration, pH, fermentation time, and stirring speed influence the fermentation process. Computational Fluid dynamics (CFD) package can be applied to observe the procedures in a fermenter. CFD simulates fluid movement, energy transport, chemical reactions, and other phenomena with the aim of clarifying their impact on the overall effectiveness of bioethanol production. In this journal, a review of the fermentation process with CFD modeling was made to look at the parameters and phenomena during the bioethanol production process. The analysis commences with an examination of the processes involved in bioethanol production and underscores the crucial role of fermentation in transforming renewable resources into bioethanol. Subsequently, it delves into the foundational principles of CFD and how they are incorporated into the modeling of bioethanol fermenters. Furthermore, the review highlights key advancements and innovations in CFD modeling techniques, such as multiphase models, turbulence modeling, and coupled simulations, aiming to capture the intricate interplay of physical and biological phenomena within fermentors. Insights into the impact of operating conditions, reactor design, and microbial behavior on bioethanol yield and quality are discussed, providing a comprehensive understanding of the complex system dynamics.

Key words: CFD, Fermentor, Bioethanol

#### **INTRODUCTION**

Growing numbers of people and industrial advancement led to an elevated reliance on fossil fuels as the predominant energy source. Fossil fuels are a significant source of carbon dioxide emissions, resulting in rising temperatures. This increase in temperature leads to many consequences such as rising sea levels, changing the climate, diminished ecology, and pollutants in metropolitan areas. Hence, discovering alternate energy sources is a viable option to address this issue. The need for renewable energy sources is consistently rising due to the increased usage of fossil fuels. This represents around 33% of wind renewable energy and 10% of hydropower. Because of their significant caloric rate (35.7 MJ L-1 for gasoline, 23.4 MJ L-1 for ethanol), liquid biofuels contribute to over 15% of greenhouse gas emissions. Consequently, a persistent aspiration exists to enhance the paths for ethanol production [1][2].

Bioethanol is a very interesting fuel source that shows potential as a viable alternative to liquid gasoline. It is derived from sustainable raw materials and is ecologically benign. Additionally, it offers significant monetary advantages and is highly lucrative. Bioethanol is an ecologically benign and sustainable biofuel [3]. Bioethanol is derived from plants and can reduce CO2 emissions by as much as 18% in comparison to emissions from fossil fuels. Bioethanol may be derived from several sources including molasses, cassava, sugar cane, sweet potato, maize, and many other substances that are rich in sugars, starches, or carbohydrates [4].

Molasses is a residue of the sugar industry which is used as a feedstock for the first-generation bioethanol. It comprises non-sugar components like acidic substances, lipids, inorganic compounds, and polymers. These components influence the naturally large thickness of molasses. Molasse is a thick liquid that, if utilized as a base, must be mixed with water to provide the optimal environment for the yeast. Hence, the amalgamation of molasses and water is a crucial element which greatly impacts the efficacy of the fermentating procedure [5]. Sugarcane molasses is a dense and black fluid that contains a high concentration of important nutrients for microbes, including C, N, P, Na, K, and non-nitrogen-bearing substances.

Received : December 2, 2023 Revised : December 13, 2023 : December 20, 2023

Fermentation methods are necessary for the generation of bioethanol from molasses. The processes included are sugarcane harvesting, molasses generation, and bioethanol synthesis via fermentation. The process of molasses manufacturing involves the steps of cleaning, preparing, grinding, and treating the concentrate. Unprocessed molasses is taken and kept in tanks. Next, molasses is transferred under pressure using electric pumps to further tanks, and additional ingredients are inserted to dilute the molasses. Subsequently, the diluted molasses is transferred to the main fermentor using a pump. Four fermentors operated continuously as a system. The level of bioethanol is gradually increased throughout the fermentation process. The fermented slurry undergoes purification and refinement using six distillation vessels [6].

Periyasamy et al. [7] found the optimized conditions to get the highest yield of bioethanol. They analyzed the molasses in fermentor for different variables such as temperature, pH, and time. Their result showed that optimum conditions are a temperature of 350 °C, pH of 4.0, and a time of 72 h that gave a highest bioethanol yield of 53%. The fermenting procedure was conducted in anaerobic conditions, and the outcomes was in comparison with the Michaelis-Menten model, and the predicted values of Vmax and Km were determined.

Currently, yeast strains available in markets may be categorized into many categories based on their kinds (such as baking, brewer's, alcohol, bioethanol, etc.), and purposes (including bakery, alcoholic drinks, drinks without alcohol, etc.). Each of these methods will yield a distinct outcome when used in the manufacturing of bioethanol. Given that each method exhibits a distinct composition, despite the use of an identical basic yeast [8].

Saccharomyces Cerevisiae is a widely recognized yeast used in brewers that can convert glucose into bioethanol in the absence of oxygen. The bacterium is well-suited for producing bioethanol since it has advantageous characteristics, which include rapid growth, effective glucose consumption, fermentation of ethanol capability, and resilience to environmental pressures which includes a significant ethanol level, a broad pH range, and limited oxygen levels. The economic efficiency and industrial feasibility of bioethanol production by Saccharomyces Cerevisiae stem from its rapid reproduction, which allows it to satisfy the demands of large-scale procedures [9].

Saccharomyces cerevisiae is the primary yeast kinds applied for commercial bioethanol creation due to its ease of handling, minimal nutritional requirements, capability to generate levels of ethanol exceeding 15%, tolerance to high sugar levels, cost-effectiveness, a small number of byproducts, osmotolerance, and high sustainability for reusing [10].

The glycolytic processes primarily provide the energy required for the growth of *Saccharomyces Cerevisiae* cells throughout bioethanol fermentation. Moreover, the process of producing ethanol using *Saccharomyces Cerevisiae* is both cost-effective and viable for use in industry. *Saccharomyces cerevisiae* has rapid reproduction, making it suitable for large

-scale pilot procedures that have high demands. The proliferation of a microbe is majorly impacted by the concantration of the medium, and the synthesis of ethanol is contingent upon the presence of cells. The exponential proliferation of *Saccharomyces Cerevisiae* in batch preparations with restricted resources leads to the synthesis of ethanol. Nevertheless, a significant amount of glucose at the beginning of the fermentating process might impede the utilization of the substrate, significantly reducing the effectiveness of fermenting. Therefore, to achieve an efficient fermentation process, the main focus is on maximizing the mix of the culture medium and variables. To satisfy the needs of the manufacturing sector, it is essential to enhance the system's efficiency and augment the ethanol output with no incurring additional production costs [9].

CFD simulations provide a detailed understanding of fluid movement, energy transport, chemical reactions, and other critical parameters within bioethanol production systems. This insight helps researchers and engineers comprehend the complex interactions occurring within fermentors, enabling a more profound understanding of the underlying processes. CFD allows for the virtual testing and optimization of different reactor designs. By simulating various configurations and operating conditions, researchers can identify the most efficient reactor design for bioethanol production. This optimization process can lead to improved performance, reduced energy consumption, and enhanced yields. CFD simulations can predict the performance of bioethanol fermentors under different scenarios. This predictive capability is valuable for assessing the impact of changes in operating conditions, such as temperature, pressure, and flow rates, on the overall efficiency and productivity of the bioethanol production process. CFD simulations enable the identification of potential issues and challenges in the bioethanol production system before actual implementation. This helps in troubleshooting and mitigating risks, saving time and resources in the experimental phase. Through virtual simulations, CFD allows for cost-efficient iterations of design changes. Instead of physically modifying equipment, researchers can test and refine different configurations in the virtual environment, reducing the need for expensive and time-consuming trialand-error experiments. CFD simulations are valuable when scaling up bioethanol production processes. They provide insights into how changes in scale may affect fluid dynamics and heat transfer, assisting in the smooth transition from laboratory-scale to industrial-scale production. CFD can be used to assess the environmental impact of bioethanol production processes by modeling emissions, energy consumption, and other factors. This information is crucial for developing sustainable and environmentally friendly bioethanol production methods [11] [12] [13].

The previous review discussed CFD in the bioethanol production process, which reviewed the hydrodynamic characteristics of the mixing behavior in the fermentor. For this reason, this review will also discuss the fermentation reaction during the bioethanol production process in the fermentor to obtain optimal conditions.

### 2. FERMENTOR

Bioreactors, such as fermentors, are crucial components in any biological procedure. Furthermore, they are regarded as the central components of bioprocesses. Bioreactors are apparatuses where chemical reactions or processes of nature take place. The bioreactor must suggest the ideal environment to meet the needs of its physical components (enzyme, microorganism, or cell) and guarantee an excellent bioprocess output. Before designing the bioprocess, it is vital to thoroughly investigate the biological mechanisms concerned. This understanding the substrate that will be alterated and the conditions that increase activity levels and promote biological conversion, ultimately leading to a higher level of the desired product. To optimize enzymatic hydrolysis, it is crucial to identify circumstances that increase enzyme activity [14].

Cylindrical fermentors and agitated fermentors are frequently employed in the fermentation procedure. The cylindrical fermentor has two types: fluidized bed reactor and fixed bed reactor. An issue arising from the fluidized bed reactor is the significant agitated resulting from catalyst degradation and dust accumulation. The fixed bed reactor is plagued by frequently unintended heat gradients, controlling the temperature challenges, and difficulties in washing or repairing. In contrast, the agitated fermentor offers the benefit of better evenly dispersed heat transfer and comparatively better mass transfer.

Agitated fermentors are vital apparatuses employed in industrial operations. Stir fermentors are often used in the industry to facilitate the circulation of fluid inside them. Agitated fermentors are often used for blending, combining several solute solutions, dispersion of different solutions that are not capable of being mixed, blending in systems that consist of many phases, and various other applications. The dimensions of the fermenter are contingent upon the chosen method, operational procedures, and the desired result. Specifically, for experimental purposes, the fermenter typically: (a) ranges from 5 to 10 liters in size; (b) the test scale requires a volume ranging from 10 to 500 liters; (c) for a significant industrial scale, the volume typically ranges from around 500 to 400,000 liters.

There is another type of fermenter, namely batch fermenter. A batch fermenter is a reactor or fermenter variant in which the fermentation process occurs within a specific single cycle or batch. Differing from continuous fermenters that operate the process continuously, batch fermenters handle a defined quantity of raw material and pause upon reaching a specific stage in the time cycle. After the completion of one cycle, raw materials are introduced, and the ultimate product is extracted prior to commencing the subsequent cycle. Batch fermenters are usually used in the aeration process [15].

#### 3. BIOETHANOL PRODUCTION PROCESS

The last step in the synthesis of bioethanol is fermentation when the monomer sugar acquired from enzymatic hydrolysis is converted to bioethanol by microbes

including yeast, bacteria, and fungus. The primary organic substances employed in bioethanol creation are yeasts, with Saccharomyces cerevisiae being the most prevalent. This yeast species can convert hexose carbohydrates, notably glucose, into ethanol via fermentation, given appropriate control over the circumstances.

The three most often used procedures in bioethanol generation are separate hydrolysis and fermentation (SHF), simultaneous saccharification and fermentation (SSF), and simultaneous saccharification and co-fermentation (SSCF). SHF segregates the process of breaking down the biomass into hydrolysis and the process of converting it into ethanol fermentation. Enzymatic saccharification fermentation are conducted unconnectedly, allowing enzymes to function at elevated temperatures to enhance their efficiency, while fermentation organisms may act at lower temperatures to maximize sugar utilization [16]. To keep the glucose content low, the enzymatic saccharification and fermentation processes accur concurrently in SSF and SSCF. SSF differentiates the fermentation of glucose from pentoses, whereas SSCF carries out the fermentation of both glucose and pentoses in a one reactor. SSF and SSCF are favored over SHF due to the ability to do the procedure in the same vessel. Both methods exhibit lower expenses, superior ethanol production, and reduced processing durations [17].

The key reactions that happen throughout fermentation are as follows:

a. The reaction breaks down sucrose into glucose and fructose

$$C_{12}H_{22}O_{11} + H_2O \xrightarrow{Zymase} 2C_6H_{12}O_6$$

b. Ethanol formation reaction.

$$C_6H_{12}O_6$$
 Invertase  $2C_2H_5OH + 2CO_2$ 

A further approach to improve the economic viability of enzymatic saccharification is the acceptable-recognized simultaneous saccharification and fermentation (SSF) method. This method involves combining enzymatic and fermentation procedures into one process, resulting in reduced expenses for devices, procedures, and manufacturing.

In a prior research studied by Fan et al. [18], the simultaneous saccharification and fermentation (SSF) technique was employed to co-ferment pretreatment sugarcane bagasse (SCB) and molasses. The ratio of SCB to molasses utilized was 3:1, and the mixture was introduced to a erlenmeyer flask. A pH was regulated to 4.5 by adding 1.0 mol L-1 sulfuric acid. Following an autoclave at a temperature of 121 °C for 20 min, precise quantities of cellulase (15 FPU g-1 pretreatment SCB) and activating yeast (5 mL) were introduced in the apparatus. To achieve a total volume of 100 mL, a certain amount of sterilized water was introduced into the blend. The fermentation process was conducted at 34 °C and 120 rpm for 120 h in a shaker apparatus. The findings indicate that the maximum level of ethanol achieved was 94.20 g L-1, which was produced when the solid dosage was set at 44%.

Furthermore, the ethanol yield was measured to be 72.37%.

### 4. OPTIMIZATION CONDITIONS FOR THE ALCOHOLIC FERMENTATION PROCESS

The pH, or hydrogen ion concentration, acts an important part in the procedure of fermentation. A pH level has an impact on the growth rate of Saccharomyces cerevisiae. Saccharomyces cerevisiae has a significant influence on the generation of ethanol when the surrounding pH levels are optimal. While significantly lowering the pH of the medium hampers the growth and metabolic activity of harmful microbes, it also diminishes the efficiency of yeast in transforming carbohydrates into ethanol, leading to a decline in ethanol output [19].

Rastogi and Shrivastava [20] used enzymes, namely alpha-amylase, and glucoamylase, to degrade cellulose present in sugarcane bagasse. Five tests were created with different pH levels to determine the influence of pH on ethanol production at a temperature of 37°C. Additionally, an additional set of five tests were made to assess the effect of temperature on ethanol output, while maintaining a constant pH level of 4.5. According to the findings, the ethanol with the greatest concentration resulted in a pH of 4.5 at 35°C. These findings indicate that a pH of 4.5 and at 35°C are the ideal circumstances for yeast to produce ethanol.

The temperature directly affects the motion of Saccharomyces cerevisiae and indirectly affects the quantities of bioethanol generated. Additionally, temperature regulates microbial activity, the pace of reaction rates, and the balance of the procedures of fermentation. The ideal temperature range for the development and metabolic activities of Saccharomyces cerevisiae is between 25 and 35 degrees Celsius. Temperature has an effect on the pace of chemical reactions through the fermentation procedure. Elevated temperatures accelerate the reaction rate, but they may also cause denaturing of proteins, damage microbes, and hinder bioethanol synthesis [21][22].

# 5. THE PRETREATMENT IMPACT ON BIOETHANOL PRODUCTION

The pretreatment stage is crucial since it significantly influences the total effectiveness of bioconversion. The pretreatment aims to degradae the resistant constructions of cellulosic material to imrpove the cellulose-access to enzymes that catalyze the conversion of carbohydrates into sugars that can be fermented. The key objective of pretreatment is to enhance the ability to digest cellulose by augmenting the availability of enzymes. To optimize the hydrolysis and fermentation stages, it is important to employ alternate pretreatment procedures and circumstances that have specific effects on the cellulose, hemicellulose, and lignin components [23][24][25].

#### a. Physical Pretreatment

Physical pretreatment techniques, such as milling, grinding, chipping, freezing, and radiation, enhance the surface area of lignocellulosic compounds while reducing the size of their particles. Moreover, it leads to a reduction in the polymer chain length and a decline in the crystalline structure of the raw material. Usually, a mixture of physical

and additional pretreatments is carried out [26][27].

Biomass materials, whether wet or dry, may be decreased in size by mechanical comminution using milling, grinding, and chipping techniques, either alone or in combinations. Comprehensive study on the impact of particle size on biomass processed has consistently shown that improvements in the procedure are linked to the capacity of pretreatment to rise the active surface area and reduce the crystalline structure of substances [24][28].

#### b. Chemical Pretreatment

The impact of alkaline pretreatments, which vary in effectiveness based on the lignin level of the biomass, is seen on the lignocellulosic biomass. Alkali pretreatments enhance the ability to break down cellulose and dissolve lignin while causing minimal cellulose and hemicellulose compared with acidic or hydrothermal methods [29].

Sulfuric acid pretreatment is the prevailing method for chemically treating biomass. This process involves hydrolyzing polysaccharides, particularly hemicelluloses, into simple sugars. As a result, the susceptibility of cellulose to enzymatic saccharification is enhanced. Acidic pretreatment may be conducted using either a lower acid level and higher temperature or a larger acid dosage and lower temperature [30].

The use of sulfuric acid for the preparation of molasses significantly influenced the fermentation procedure carried out by *S. cerevisiae Y17*. Pretreating molasses with sulfuric acid achieved significant ethanol production (8.55%). Alternatively, using nitric and phosphoric acids during the pretreatment phase increased the generation of ethanol by 8.06% and 7.51% respectively [31].

The earlier study investigated by Jayanti et al. [32], described that the bioethanol generation of molasses medium employing instantaneous dry yeast Saccharomyces Cerevisiae is greatly influenced by the pre-treatment procedure including sulfuric acid and the fermentation temperature. As measured by the Multiple Attribute Test, the optimal pretreatment involved using a molasses slurry with sulfuric acid treatment at 32 °C. This treatment resulted in a substantial drop in whole solvable solid by 10.9 % Brix, a reduction in sugar levels by 12.15%, an intake of reduced sugars by 57.21 g L-1, an bioethanol level of 8.30%, and the yield of 68.67%. The fermentation temperature affects the ethanol concentration. The enzyme activity and rigidity of the yeast cell membrane are greatly influenced by temperature. Elevated temperatures during fermentation may decrease its efficiency.

# c. Physiochemical Pretreatment

Steam explosion is the prevailing physicochemical processing technique for biomass. Hydrothermal treatment involves subjecting the biomass to pressured steam for a brief duration, between seconds to several minutes, followed by depressurization. This pretreatment involves the combined mechanical and chemical forces resulting from the autohydrolysis of acetyl links in hemicellulose [33].

#### d. Biological Pretreatment

Biological or microbiological pretreatment, in contrast to chemical and physicochemical pretreatment techniques,

does not need the use of any chemicals. This pretreatment method is ecologically sustainable and involves the use of microbes, in particular fungal organisms, to transform lignocellulosic biomass into chemicals that are easier to break down by hydrolysis and may be used for the synthesis of bioethanol [34].

# 5.1 Effect of Different Molasses Sugar Concentrations on Bioethanol

The highest bioethanol yield was obtained while the sugar content was between 15% and 20% of molasses [35]. In addition, a procedure for screening was carried out to ascertain the precise amount of sugar in molasses. This screening included testing at 1% increments within the range of 15% to 20%. Subsequent rises in sugar molasses content led to a decline in bioethanol output. Zentou et al. [35] examined the impact of several operational parameters on the output of fermentation. The analysis revealed that the most favorable parameters for molasses fermentation were a pH of 4.5 at 30 °C, and a substrate concentration of 50 g L<sup>-1</sup>. It is evident that the acidic environment is conducive to the activity; so, one may assert that Saccharomyces Cerevisiae yeast is an acidophilic microbe. Additionally, the low pH level is conducive to the breakdown of sucrose into fermentable sugars by the invertase enzyme. The yeast's physiological characteristics primarily determine the ideal sugar concentration. A high sugar concentration can result in a greater extracellular is the term osmotic pressure compared to intracellular circumstances. This causes water within the cell to flow across a membrane.

# 6. COMPUTATIONAL FLUID DYNAMIC

Computational Fluid Dynamics (CFD) is the study and modeling of fluid flow, heat transport, and associated phenomena including chemical responses utilizing computer -based analyses. CFD offers more flexibility for modifying vessel layout and size, propeller direction and speed, as well as hydrodynamic characteristics. A CFD code consists of computational techniques designed to handle issues related to fluid flow.

The majority of current CFD simulations for the generation of bioethanol were specifically developed to mimic the process of biomass fermentation in agitated vessels. A single study on a cylindrical reactor with a perpendicular input has been conducted. Nevertheless, only a few of these investigations took into account a kinetic simulation for the fermentation process. In future versions, it is possible to implement intricate kinetic systems to accurately depict the rate of bioethanol synthesis. It is possible to simulate additional sophisticated methods for generating bioethanols, including simultaneous hydrolysis and fermentation using enzymes. The Euler-Lagrange approach is applicable in this instance [11].

Precisely forecasting the hydrodynamic characteristics of reactors of different dimensions and how they connect with organisms is crucial in most bioprocesses. Computational fluid dynamics can accurately simulate hydrodynamics and dispersion [36]. CFD (computational fluid dynamics) has been used to simulate upward

bioprocessing stages, including fermentation and homogeneity. CFD studies have often been used to analyze the flow of a single phase and the resulting hydrodynamic stress. Nevertheless, actual bioprocessing actions include the presence of a minimum of two distinct phases, namely cells and liquid. The gas bubbles represent the third phase inside the bioreactor. The latest computational fluid dynamics (CFD) simulations have included the consideration of motion and the transfer of masses that occurs among the different phases [37].

CFD enables the modeling of the hydrodynamics of huge-scale bioreactors and offers a comprehensive understanding of the microbiological ecology inside fermentors [38]. Computational Fluid Dynamics (CFD) encompasses many phenomena related to the motion of fluids, including two-phase fluid systems, the mass and heat transport, chemical processes, the dispersed behavior of gases, and the motion of particles in suspension. The CFD system typically consists of relevant transport equations, specification of appropriate boundary conditions, and choosing or creation of computer algorithms to execute the computational techniques applied. A CFD code consists of a computational approach capable of uncovering fluid flow issues. A Computational Fluid Dynamics (CFD) code has three primary element steps: a pre-processing, a solving, and a post-processing. Pre-processing is feeding the flow problem into a Computational Fluid Dynamics (CFD) software. This procedure includes converting the data being input to the appropriate type from the solver to utilize.

Mathematical models and computer simulations are useful means of devising techniques to enhance the extraction of energy from materials. While desktops grow increasingly powerful, simulation methods like CFD are becoming less costly and more readily available. CFD approaches can depict many phenomena that prove challenging to explain using standard mathematical frameworks relying on partial differential equations. Conventional designs for packed-bed SSF reactors have not taken into account the possibility of heterogeneity compaction of the substrate throughout bed load. The dispersion of permeability may impact the transport of energy and mass, thereby influencing the development of biomass. CFD simulations cannot just depict uneven flow patterns of distribution but also manage intricate bioreactor shapes and the existence of flow impediments [39].

Originally, water was employed to facilitate the movement within the bioreactor. The Navier-Stokes equations are expressed as a set of mathematical formulas. The simulation formulas employed were (1) and (2).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$
 (1)

$$\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U X U) = -\nabla p + \nabla \tau + S N \tag{2}$$

Where  $\tau$ :

$$\tau = \mu \left( \nabla \mathbf{U} + (\nabla \mathbf{U})^T - \frac{2}{3} \partial \nabla \cdot \mathbf{U} \right)$$
 (3)

U is the velocity, p the pressure, t the time,  $\rho$  de density, and SN the driving forces [40].

The CFD code consists of computational methods designed to tackle issues related to fluid flow. A CFD code has three primary stages: a pre-processing, a solving, and a post-processing. Pre-processing is inputting the flow problems to a CFD application and converting it to a format that is appropriate for the solver to utilize.

The stages involved in the current phase are as follows: (1) Establishing the precise characteristics of the geometry being evaluated; (2) Generating a grid, which involves dividing the domain space into non-overlapping smaller components; (3) Identifying the specific physical forces that require to be modeled; (4) Defining the characteristics of the fluid being studied; (5) Selecting the boundary conditions for the control volume or cells which align along the domain's boundary region; (6) Solving flow problems, such as determining the velocity, pressure, and temperature at the cell locations within each node. The precision of CFD settling is contingent upon the quantity of cells in the grid. The Solver may be categorized into three distinct kinds: finite difference, finite element, finite volume, and spectral approaches.

ANSYS FLUENT resolves governing equations for all streams. In cases when heat transport and compressibile fluid is involved, the extra equation for energy transfer is addressed. In cases when there is a combination of species or chemical processes, a species conservation equation is calculated. If the flow is turbulence condition, extra transport equations are also resolved. In this study, isothermal situations are specifically selected, resulting in the solution of solely hydrodynamic problems [41].

Prior research has concentrated on the mixing properties inside agitated vessels. For example, a CFD-based model was introduced to determine the mixing circumstances in bioethanol fermentors. The simulation results indicate that the flow patterns within the impeller and along the tank wall exhibit a circulating loop and a fluctuating flow pattern, respectively. The duration of mixing for the impeller rotating at 1300 rpm is 29.1 seconds, while for 1600 rpm, it is 19.2 seconds. The homogeneous index value is 0.9224. During a 30-second mixing period, the highest homogeneity index value recorded was 0.9237 for the parameter of the speed of rotation set at 1300 rpm, whereas the highest homogeneity index value recorded was 0.9832 for the variable of rotating speed set at 1600 rpm.

A prior study [42], conducted a CFD model of a 70 m³ commercial fermentor using an Eulerian approach. The physical parameters of a 0.25-weight percent liquid xanthan solution were determined with a bubble size of 2 millimeters. The multiphase mass transfer was simulated using the two-film concept and simple Maxwell-Stefan multicomponent dispersion. The model involved the bioreaction kinetics of xanthan gums. The process of local mass transfer and bioreaction was mathematically represented, and the dispersion of gaseous NH³ and liquid nutrition was performed as well. The advanced reactor design accurately indicates possible areas of concern inside the fermentor [42]. The findings demonstrated a notable variation in the

local response and circumstances of mass transfer. The simulation findings indicate that phenomenology models and tests enable the examination of specific reactions and mass movement between gas and liquid in stirred fermenters. Incorporating population balances for bubbles might enhance the accuracy of predicting local situations.

CFD was employed by other researchers [43] to model a fermentor that involves gas, liquid, and solid phases. A hydrodynamics with reaction kinetics schemewas created using CFD software to model a multiphase pretreatment process. The investigation revealed the visualization of flow patterns and the evaluation of critical factors. The linked models also illustrate a qualitative correlation among hydrodynamics and hydrogen generation, emphasizing that the regulation of hydraulic retention time (HRT) is a crucial determinant in hydrogen production. This approach is appropriate for schemes that have a continuously flow movement, however it is difficult to be used for process that operate in batches or have highly unpredictable hydrodynamic behavior without substantial changes to the model [43].

Um and Hanley [44] conducted a study on developing a high-concentration medium movement apparatus for this procedure. They utilized the commercially available CFD package Fluent to assess the effectiveness of different bioreactor designs and analyze the flow distribution and associated phenomenon in the small-scale reactor. The physical model used to simulate a stirred tank with a Rushton propeller comprises an ellipsoidal, circular vessel with four evenly spaced baffles attached to the walls. These baffles reach from the vessel bottom to the free surface. The tank is agitated by a 6-blade Rushton turbine impeller, which is placed in the center. The findings indicate the possibility of reduced or inactive movement among the upper impellers and the lower part of the tank area, leading to inadequate transport of nitrogen and temperature for fermentations with high viscosity. The findings also indicate a substantial increase in the axial velocity for the altered configuration at the lower section of the tank.

In a 2019 case study conducted by Shu et al. [45], the CFD-Taguchi approach was used to examine the impact of control parameters, including propeller kind, flow of gas rate, and agitating velocity, on gas holdup and energy use during Aureobasidium pullulan fermentation in a agitated fermentor. The investigation yielded three distinct viscosities, which were designated as control variables based on the growth graph of viscosity seen throughout fermentation. Following that, the quantitative assessment of control variables in the fermentation procedure was conducted. The biomass level of Aureobasidium pullulans showed a correlation with the uniformity index K and the stream behavior index n. Additionally, the uniformity index was shown to be connected with the length of the fermentation period. Enhanced methods of fermentation and control strategies may be devised to facilitate the energyefficient manufacturing of Pullulan and enhance the cleanliness of the aerobic fermentation technique. The next study should prioritize the investigation of the multiviscosity phases of Aureobasidium pullulans fermentating and other

microbial type.

Carvajal et al. [46] demonstrated time-dependent modifications in the rheological properties of pretreated Arundo utilizing steam explosion throughout enzymatic saccharification. These changes were calculated based on laboratory results that were further analyzed by CFD models, with the Herschel Bulkley model used as the rheological theory. The three-parameter Herschel Bulkley model may accurately illustrate the rheological performance of prepared Arundo slurries throughout enzymatic saccharification, namely the change from shear-deepening to Newtonian performance. The analysis of the Herschel Bulkley variables indicates that the stress yield diminishes by time as the number of solids lowers. Still, the consistency index rises, indicating a shift in the physicochemical properties of the mixture. The decline in the stream performance's index over time, eventually approaching or falling below unity, is a result of the shift from shearthickening behavior to a Newtonian behavior.

The work conducted by Wu [47] assesses six turbulence equations for the motorized stirring of non-Newtonian liquids in a laboratory-scale biodigestion reactor using a pitched blade turbine (PBT) propeller. The approaches under investigation include the standard k- $\epsilon$ , the RNG k- $\epsilon$ , the realizable k- $\epsilon$ , the standard k- $\epsilon$ , the SST k- $\epsilon$ , and the Reynolds stress models. The use of a second-order discretization technique for the momentum equations enhances the reliability of movement value estimation but has a detrimental impact on the precision of the power numbers. The sliding mesh technique often outperforms the MRF approach in accurately estimating power and flow values. Nevertheless, it necessitates a significantly extended duration for computation [47].

The study conducted by Li et al. [48] demonstrates that achieving a consistent distribution of slurry over a prolonged period is crucial for enhancing performance. An attempt was undertaken to create a new quasi plug flow reactor on a large scale for enzymatic saccharification of cellulose using CFD modeling. Before conducting computational modeling, the rheological characteristics of the cellulose enzymolysis mixture derived from furfural wastes were investigated by experimental analysis. A turbulence type known as k-ke was used in the numerical study, demonstrating proficiency in characterizing the flow pattern with notable fluctuations in the magnitude of turbulence inside the agitated tank. Initially, an investigation was conducted on vertical and pitched blades, helical ribbons, and the combination. Subsequently, the inside components were optimized. The RTD graph calculation revealed that the quasi-plug flow reactor included the subsequent characteristics: (1) it consisted of a mixture of double-helical ribbons and vertical blades; (2) it had two sections and four baffles; (3) the flow surface on the partitions measured 0.1 m2. In terms of power usage, the helical ribbon had the lowest power consumption, next by the pitched blade and vertical blade. The integration of double-helical ribbons and vertical blades in the impellers effectively resolved the issues of lower velocity and higher viscosity. The required duration for the residence period exceeds the duration for achieving mixing in the reactor. Changing the impeller design [48] did not allow for the achievement of plug flow.

With work undertaken by Bach et al., [49], simulation was performed on agitated reactors to create and build up procedures for bioreactors. There is a baffled bioreactor in the shape of a torispherical bottomed tubular tank with a liquid depth ranging from height of 0.7-1.65T, that generates an input volume ranging from 150-350 liters. The blending duration for a single stage is established by a combination of air (Newtonian) and Xanthan Gum solution (non-Newtonian) with different levels. Mass transfer constants were chosen from six Trichoderma reesei fermentation under established process parameters. Additionally, the mass transfer estimated by the Higbie penetration concept of twophase CFD calculations leverages a relationship between bubble size and power input, and the total mass transfer factor is in excellent accord with the actual results. The mixing parameters of air and Xanthan gum were satisfactorily predicted, with blending power varying between 0.5 to 9.2 kW m<sup>-3</sup>. The indirect approach was constructed to compute the fermenter bubble size by analyzing the data. The inlet flow rate and power input for circumstances that determine bubble size. This study has proven how to utilize and create CFD simulations using procedure information from commercial fed-batch fermentation. The CFD models and resulting relationships may be utilized when using biological frameworks to analyze substrate diffusion and absorption rates.

A study was conducted to evaluate the efficiency of a new kind of propeller called "narcissus" in a tripled propeller bioreactor. The study used a 3D networks-of-zones concept to illustrate the mixing of liquids procedure. Modifying the volume of certain zones provides a rapid means of replicating the three-dimensional up-down flow structure of the NS propeller in simulations. The mass balance calculations for all zones remain unchanged. The simulation was constructed via a 3 x 2 x (10 x 10) x 60 arrangement to replicate the outcomes of pilot plant three-propeller experiments, employing the identical Tylosin reaction that had been employed in Rushton turbine studies. The gas volume, oxygen gas, and oxygen liquid mass fraction dissolution may be shown as solid-body domains in a 3D complicated perspective. The domain of reaction rate for depicted simple-ordered kinetics has comparable challenges. If employed in the triple structure, the NS impellers are yield anticipated to greater dissolved concentrations in the immediate vicinity compared to Rushton turbines [50].

CFD method was created to analyze the behavior of yeast enclosed in capsules. This method aimed to understand the properties of encapsulating yeast utilized in ethanol production from lignocellulose waste. Encapsulated yeast is a physiologically active substance that is protected by a semipermeable barrier to prevent inhibitor damage to cells. The encapsulating yeast method focuses on the efficient transport of substrate (glucose) through and out of the

Table 1 Several CFD Modeling Research

No.	Topic	Models and Condition	Computational Details	Findings
1.	Investigation of the molasses-water mixing dynamics in an ethanol bioreactor. Experimental investigations and CFD simulations [5].	Case: Investigation and CFD simulation of the mixing dynamics between molasses and water in a agitated tank. Phases treatment: Single phase Turbulence: κ-ε model Rheology Conditions: Transient - Impeller velocity 1000 to 1300 rpm.	CFD Code: ANSYS Fluent 18.2.  Geometries: a cylindrical cone-shaped stirred tank (3D).  Mesh: Unstructured tetrahedral mesh Solution method: NA	The experimental findings on mixing behavior revealed that the molasses and water combination exhibited three distinct zone processes, namely the rheological characteristics and impeller rotating velocity. These elements were shown to have the most influence. Furthermore, the use of the Eulerian multiphase model and Large Eddy Simulation may be employed to forecast the blending characteristics in large-scale agitated bioreactors used in industry.
2.	CFD Analysis of Modified Rushton Turbine Impeller [53]	Case: Determining the optimal inputs in the cylindrical stirred tank by varying the blade angles Phase treatment: Single phase Turbulent: κ-ε model Conditions: Impeller velocity 120 rpm.	CFD Code: NA Geometries: A cylindrical tank with four-bladed rushtone turbine impeller Mesh: NA Solution method: NA	Based on the findings, the power number exhibits a 30% increase when the RTI-45° upward eccentric position is considered, concurrently with an 11% elevation in the flow number. Conversely, the power number is lower when the RTI-10° and 20° are applied in the upward eccentric position, with the flow number remaining consistent compared to the Rushton turbine impeller.
3.	CFD simulation is developed to accurately forecast the flow fields of highly viscous fluids in a reactor across different operational scenarios [44].	Case: Fluid flow throuhout the fermentating of cellulosic slurry Phases treatment: NA Turbulence: $\kappa$ - $\epsilon$ model Conditions: Initial solids concentration 10 to 20% (w/ v); propeller speed of 120 rpm	CFD code: Fluent 6.2.20 Geometries: A 3-Litres of vessel with 4- equidistant wall- mounted baffles and two centrally located 6-blade Rushton propellers (3- D) Mesh: Unstructured tetrahedral mesh Solu- tion method: NA	Regions characterized by elevated shear forces inside the bioreactor facilitate a decrease in the viscosity of the entire system. A direct correlation among the level of solids and the perceived viscosity was discovered.

capsule, as well as the fermentation process. The purpose of mass transfer simulation is to enhance our understanding of capsule effectiveness, which encompasses three key elements: cell grouping, liquid distance, and thinner membranes. In essence, the magnitude of the glucose mass flow is inversely proportional to the thickness of the membrane. The findings demonstrate the presence of a gradient in glucose levels inside the cellular solid domain, suggesting that the reaction has an impact on it. This is apparent from the level of glucose profile in both the solid and liquid domains of the cell. The membrane region where the cells are joined has a greater concentration than the liquid portion [51].

The modifications were made to the Eulerian two-fluid system frameworks to approximate the synthesis of enzymes by the filament fungal T. reesei. An Eulerian multiphase technique was employed to impact fermentation. Initially, the computerized simulation was verified by comparing it to measurements that had been earlier gathered in viscous non-

Newtonian liquids. The use of the persistent Multiple Reference Frame method, in combination with periodic boundaries. The general drag rules were applied specifically in air-water models, resulting in a 10% error in predicting the gas holdup and a 14% error in predicting the Relative Power Demand. The existence of substrate and the rate at which it is produced varied among the bigger reactors beneath those circumstances. The bigger bioreactors were decided by the gradients of substrate and output rate beneath these circumstances. Upon doubling the feed flow rates, the response period for every setup significantly exceeded the circulation time. Consequently, the nutritional content was evenly dispersed within the fermenter. Simultaneously, the elevated substrate load resulted in a rise in the need for oxygen, leading to a decrease in the remaining oxygen level. Consequently, the bigger tanks functioned in circumstances where there was a restricted supply of oxygen, leading to a drop in the effectiveness of the fermenter [52].

Table 1 is a compilation of many research conducted on CFD Simulation, each addressing various challenges. The conducted tests have shown that the simulation can accurately describe the mixing behavior occurring in the stirred tank throughout the entirety of the bioethanol manufacturing procedure. CFD may be used to analyze the impact of variations in stirring speed and feed concentration in large-scale stirred tanks used in process industries. The objective of Madhania et al. [5] research is to examine the mixing characteristics of molasses-water in a cylinder coneshaped mixing vessel system, specifically focusing on the impact of molasses-water rheological features. The experimental findings indicate that the molasses-water combination exhibits three distinct zone processes, with the rheological characteristics and impeller rotating speed being the most important elements.

#### 7. CONCLUSION

In this paper, we present various uses of CFD in the bioethanol production process. CFD is used for modeling and continuous improvement to produce bioethanol with an efficient process with maximum yields. CFD can describe the bioethanol production process, such as flow patterns, mass transfer, energy, and chemical reactions. From the various studies that have been reviewed, CFD research that focuses on chemical reaction modeling has not been widely applied. The final recommendations from this paper can be a challenge and an opportunity for progress in research development in the bioethanol production process.

#### AUTHOR INFROMATION

#### **Corresponding Author**

\*Email: alistria97@gmail.com \*Email: novia@ft.unsri.ac.id

#### ORCID (D)

Novia : 0000-0002-0046-6076 Fitri Hadiah : 0000-0002-4222-2352 Ali Satria Wijaya : 0009-0003-4790-7531

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