Chapter 15

Introduction to computational fluid dynamics in airlift bioreactors for ethanol production: a review

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ABSTRACT
There is a growing number of studies related to computational fluid dynamics for the construction and optimization of equipment, machines, and systems. In this work, the main knowledge needed to perform an analysis of computational fluid dynamics in airlift-type bioreactors for ethanol production will be addressed.

Keywords: biofuel, airlift bioreactor, ethanol, computational fluid dynamics.

1 INTRODUCTION

According to the Ministry of Infrastructure, by December 2020, Brazil had 109,773,263 vehicles, of which 58,184,427 are cars (MINISTÉRIO DA INFRASTRUCTURA, 2021). Of these, there was the following number/category of cars: 30,316,743 alcohol/gasoline, 22,108,306 gasoline, 3,756,070 alcohol, 966,240 gasoline/alcohol/natural gas, 884,083 gasoline/natural gas, 34,954 diesel, 13,728 gasoline/alcohol/electric, 13,590 gasoline/electric, 1,157 electric/external source, 380 electric/internal source, 89,176 other vehicles (MINISTÉRIO DA INFRASTRUCTURA, 2021).

According to previous data, it can be seen that a large portion of the Brazilian fleet is powered by fossil fuels. However, it appears that there is interest in the use of biofuels in vehicles so that there is an attenuation of external dependence on oil and the reduction of local pollution generated by vehicle emissions (LEITE; LEAL, 2007).

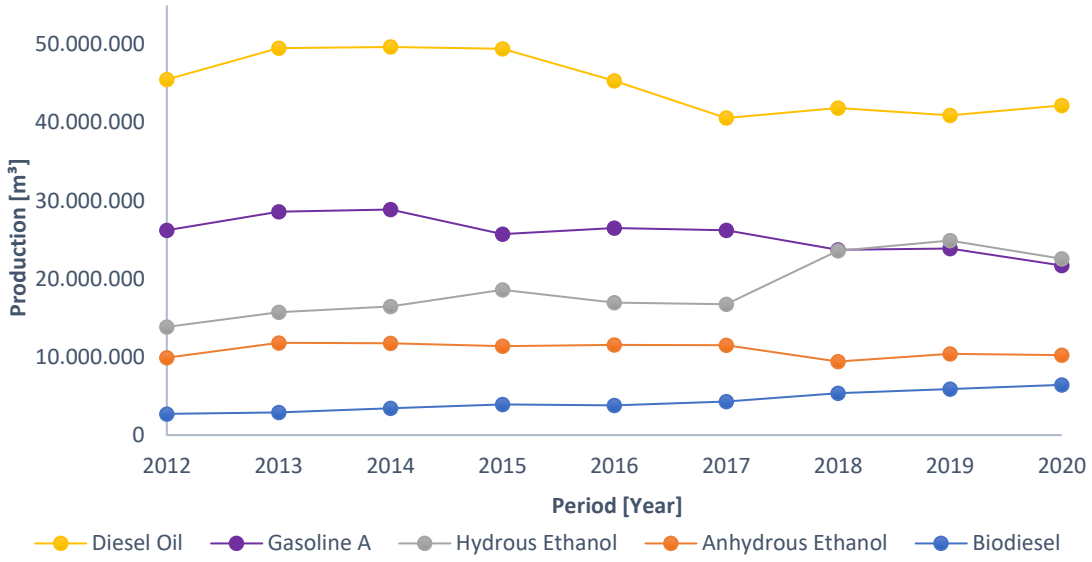
To increase ethanol production in the country, the legislation encourages the production of biofuels. With Decree 76,593 of November 14, 1975, the National Alcohol Program was instituted, to encourage the production of ethanol in Brazil (BRASIL, 1975). Zavarise et al. (2021) describe that this was an initiative of the Brazilian government to face the 1973 oil crisis and that the main objective of the program was to replace gasoline with ethanol.

Still, there is legislation that requires the addition of ethanol to gasoline. According to Law No. 13,033/2014, automotive gasoline sold in Brazil must have an anhydrous ethanol content between 18% and 27.5% by volume (AGÊNCIA NACIONAL DO PETRÓLEO, GÁS NATURAL E BIOCOMBUSTÍVEIS, 2017; PETRÓLEO BRASILEIRO S.A., 2019). The mandatory percentage of anhydrous ethanol mixed

with gasoline varied as follows: 20% from October/2011 to April/2013, 25% from May/2013 to March 15/2015, and 27% from March 15/2015 to the current date (AGÊNCIA NACIONAL DO PETRÓLEO, GÁS NATURAL E BIOCOMBUSTÍVEIS, 2017).

According to Pacheco (2011), ethanol production in Brazil is prominent, since it has advantages in production technology, in addition to the probability of leadership in energy agriculture and the biofuels market. However, ethanol production is still low compared to diesel production (Figure 1).

Figure 1: Production of Petroleum Products and Biofuels 2012-2020.



Source: AGÊNCIA NACIONAL DO PETRÓLEO, GÁS NATURAL E BIOCOMBUSTÍVEIS, 2021. Adapted.

According to Figure 1, in 2020, 42,215,122 m3 of diesel oil, 21,705,323 m3 of gasoline, 22,553,666 m3 of hydrous ethanol, 10,249,524 m3 of anhydrous ethanol, and 6,432,008 m3 of biodiesel were produced (AGÊNCIA NACIONAL DO PETRÓLEO, GÁS NATURAL E BIOCOMBUSTÍVEIS, 2021).

Among the products shown in Figure 1, the one that is mostly produced in the country is diesel oil. This, in turn, is equivalent to about 40.92% of the production of these products in 2020. Diesel oil plays a significant role in public road transport (SILVA et al., 2013) and road freight transport in Brazil (SILVA, 2010).

2 MATERIALS ANDA METHODS

The elaboration of this text was based on exploratory documentary research, through the collection of data from articles and scientific works. Thus, this work will present the basic content for understanding computational fluid dynamics (CFD) in airlift bioreactors for ethanol production.

3 RESULTS AND DISCUSSION

Several authors have carried out CFD analyses for optimizing bioreactors. In this section, the basic knowledge needed to start a CFD simulation in an airlift bioreactor applied to ethanol production will be explained.

3.1 BIOREACTOR AIRLIFT

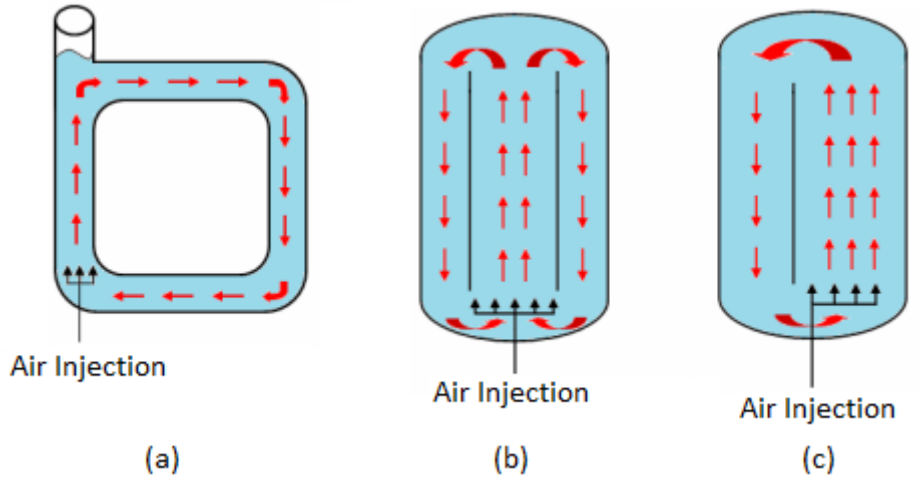
The biochemical reactor or bioreactor is a fermenter, a place where chemical reactions accelerated by biocatalysts (enzymes or whole cells) take place (SOUSA, 2016). These bioreactors have the function of promoting a controlled environment that leads to efficient cell growth (SOUSA, 2016).

Among the various types of bioreactors is the pneumatic airlift bioreactor. In this equipment, the flow of fluid is cyclic and occurs within channels: riser, where the fluid flows upwards; downcomer, where the fluid flows downwards; gas-liquid separator, which is located at the upper end of the bioreactor and connects the riser to the downcomer; and the base, which is located at the lower end of the bioreactor and makes the connection between the riser and the downcomer (ESPERANÇA, 2014).

This class of bioreactor is usually divided into two types: internal circulation airlift, where the ascending and descending regions of the fluid are in the same distribution; and airlift with external circulation, where the ascending and descending regions of the fluid are in separate partitions (ESPERANÇA, 2014) (Figure 2).

It should be noted that in the external circulation airlift, an almost total release of gas is generated in the mixing region, which consequently causes a large difference in density between the riser and the downcomer (ESPERANÇA, 2014). As a result, there is little gas circulation and a high liquid circulation speed (ESPERANÇA, 2014).

Figure 2: Types of Airlift Bioreactors.



Source: ESPERANÇA, 2014.

Legenda:
(a) *Airlift* of External Circulation.
(b) *Airlift* of Internal Circulation - Concentric Cylinders.
(c) *Airlift* of Internal Circulation - Deflector Plate.

3.2 COMPUTATIONAL FLUID DYNAMICS

CFD can be described as the branch of science concerned with the numerical simulation of fluid flow. Pessoa (2016) describes that the objective of performing a CFD simulation, in a given system and for specific boundary conditions, is to know how the fluid flow behaves.

3.2.1 Simulation Steps

The simulation can be divided into three main stages: pre-processing, processing, and post-processing (ANSONI, 2015). These steps are described below in a CFD code context.

3.2.1.1 Pre-Processing

According to Ansoni (2015), pre-processing includes the following steps: definition of the geometry, generation of the mesh, selection of chemical and physical properties, definition of fluid properties, and specification of boundary conditions. At the end of the pre-processing, there is a file with all the problem information (RODRIGUEZ, 2015).

3.2.1.2 Processing or Solver

In this step, the software reads the data file generated in the pre-processing and solves the governing equations (RODRIGUEZ, 2015). The resolution is obtained using discretization techniques: finite differences, finite elements, finite volumes, and spectral methods (ANSONI, 2015).

3.2.1.3 Post-Processing

In post-processing, the results generated by the solver are read and converted into visually interpretable data: graphs, contour maps, vector fields, and complex animations (RODRIGUEZ, 2015).

3.2.2 Computational Techniques for Modeling Interfaces

Fluid flow can develop between fluid-fluid and fluid-solid interfaces. Interface modeling can be performed by Lagrangian, Eulerian, and Eulerian-Lagrangian methods.

3.2.2.1 Método Lagrangeano

No método Lagrangeano a malha é móvel, isto é, a malha se move junto com o escoamento (MARIANI, 2002; NOLETO, 2010).

3.2.2.2 Lagrangian method

In the Eulerian method, the mesh is fixed (MARIANI, 2002; NOLETO, 2010). Models of the VOF (Volume of Fluid) type (NOLETO, 2010) and Mixture Model (BORGES, 2021) are representative of this method.

3.2.2.3 Eulerian-Lagrangian method

The Eulerian-Lagrangian method includes different approaches for the flow, the mobile geometry, and the mesh (NOLETO, 2010). The Immersed Moving Frontier method and the Arbitrary Eulerian-Lagrangian scheme are representative of this method (NOLETO, 2010).

3.2.3 Turbulence Modeling

Most flows are turbulent and with a high Reynolds number (COSTA, 2018). Therefore, it is important to use turbulence modeling for CFD simulation. According to Costa (2018), three turbulence models can be highlighted: DNS (Direct Numerical Simulation), LES (Large Eddy Simulation), and RANS (Reynolds Averaged Navier-Stocks).

3.2.3.1 Direct Numerical Simulation

In the DNS approach, the small and large scales of turbulence are solved using the Navier-Stocks equations (LIMA, 2013; COSTA, 2018). This method requires high mesh refinement, in the order of (ReT)9/4 and small time steps $\Delta t \sim (ReT)^{-1/2}$ (COSTA, 2018). Therefore, this method is indicated only for flow in simple geometries and with low Reynolds numbers (LIMA, 2013).

3.2.3.2 Large Eddy Simulation

In this method, the large turbulence scales are solved from the Navier-Stocks equations, while the small turbulence scales are solved by simple algebraic models (sub-grid model) (LIMA, 2013).

3.2.3.3 Reynolds Averaged Navier-Stocks

According to Oliveira et al. (2004), this is the most usual and practical existing method. In the RANS approach, the variables of the Navier-Stocks equations are decomposed into an average value and a fluctuation associated with turbulence (SOUZA et al., 2011; LIMA, 2013).

This method can be classified according to the characteristics of its equations: zero equation models, one equation models, two-equation models (k-ω, k-ε, k-ω SST models), algebraic models for the Reynolds and models for the Reynolds tensor (COSTA, 2018).

3.3 HYDRODYNAMIC PARAMETERS

There are hydrodynamic parameters that determine the performance related to fluid flow (ESPERANÇA, 2014). The main parameters that influence the performance of the fluid in the airlift bioreactor are described below.

3.3.1 Gas Surface Velocity

The only operational variable available in pneumatic bioreactors is the surface velocity of the gas rise. This variable, in turn, is defined below (CERRI, 2009; ESPERANÇA, 2014):

$$U_{GR} = \frac{Q_G}{A_R} \quad (1)$$

Where,
UGR: superficial gas velocity in the upwelling region;
QG: volumetric gas flow;
AR: cross-sectional area in the uphill region.

3.3.2 Gas Retention

Gas retention can be defined as the volumetric gas fraction in the gas-liquid dispersion while aeration occurs in the bioreactor (CERRI, 2009; HOPE, 2014). There are the overall gaseous retention, the gaseous retention in the upstream region, and the gaseous retention in the downstream region (CERRI, 2009, ESPERANÇA, 2014). Global gas retention is defined below (CERRI, 2009; ESPERANÇA, 2014):

$$\varepsilon_G = \frac{v_G}{v_G + v_L} \quad (2)$$

where,
ε_G: overall gas retention;
v_G: gas volume;
v_L: liquid volume.

3.3.3 Average Circulation Surface Speed

The difference in densities between the fluid in the uphill and downhill regions is responsible for the fluid circulation in airlift bioreactors (CERRI, 2009; ESPERANÇA, 2014). The average superficial circulation velocity is defined below (CERRI, 2009; ESPERANÇA, 2014):

$$U_L = \frac{x_c}{t_c} \quad (3)$$

where,
U_L: average surface speed of circulation;
x_c: path taken by a volume of fluid in one revolution;
t_c: circulation time.

3.3.4 Liquid Surface Velocity and Liquid Interstitial Velocity

The surface velocity of the liquid is different from the interstitial velocity of the liquid, since the liquid occupies a portion of the outflow channel, while the gas occupies the other portion of the outflow channel (CERRI, 2009; ESPERANÇA, 2014). The surface velocity of the liquid and the interstitial velocity of the liquid are related by the following equations (CERRI, 2009; ESPERANÇA, 2014):

$$V_{LR} = \frac{U_{LR}}{1 - \varepsilon_R} \quad (4)$$

where,
V_{LR}: interstitial liquid velocity in the ascent region;
U_{LR}: surface velocity of the liquid in the upwelling region;
ε_R: gas retention in the ascent region.

$$V_{LD} = \frac{U_{LD}}{1 - \varepsilon_D} \quad (5)$$

where,
V_{LD}: interstitial liquid velocity in the descending region;
U_{LD}: surface velocity of the liquid in the descent region;
ε_D: gas retention in the descending region.

3.3.5 Mixing Time

Mixing time is the precise time for the mixing of a substance in the bioreactor to occur (CERRI, 2009; ESPERANÇA, 2014). This variable is found through a pulse-type test and is affected by radial and axial mixing and flow effects (CERRI, 2009).

3.3.6 Circulation Time

The circulation time is the precise time for a volume element to complete one turn in the bioreactor (CERRI, 2009; ESPERANÇA, 2014). This variable is found in the mean circulation superficial velocity equation.

3.3.7 Circulation Regimes

Esperança (2014) describes two circulation regimes: the first is the homogeneous regime, where there is a low gas feed flow, providing a uniform distribution of small bubbles, with a high mass transfer rate; the second is the heterogeneous regime, where there is an increase in the gas feed flow or an increase in the reactor diameter, providing the presence of bubbles of various sizes (turbulent regime).

3.3.8 Shear Speed

An adequate shear velocity value is essential for sufficient heat and mass transfers and for cell disruption not to occur due to high velocity (CERRI, 2009). Esperança (2014) describes the average shear velocity for a range of 0.04 < UG < 0.10 m.s-1 as equivalent to:

$$\dot{\gamma}_m = 5000 \cdot U_G \quad (6)$$

where
$\dot{\gamma}_m$: average shear velocity;
U_G: surface velocity of the gas

While, the shear velocity for a range of 0.008 < UG < 0.04 m.s-1 is equivalent to (ESPERANÇA, 2014):

$$\dot{\gamma} = 1000 \cdot {U_G}^{0,5} \quad (7)$$

where
γ̇: shear speed.

3.3.9 Bubble Diameter

The place where the bubbles are generated and the rest of the bioreactor have different distributions and sizes of bubbles (CERRI, 2009). Bubble diameter is affected by sprinkler type, gas flow rate, liquid properties, and impeller power.

3.4 CASE STUDIES

In this section, the methodologies and results obtained from studies on airlift bioreactors will be presented, as shown in Table 1. Thus, the data in Table 1 can be used as a basis to carry out subsequent studies on the instrument.

Table 1: Case studies.

Methodology	Results	Reference
Studies of liquid circulation and mixing characteristics of airlift contactors.	The linear velocity of the circulating liquid is proportional to the cube root of the surface velocity of the riser gas. Still, such speed is dependent on the AD/AR geometric parameter.	BELLO; ROBINSON; MOO-YOUNG, 1984.
Study of liquid circulation in airlift reactors.	The liquid circulation rate increases with the square root of the reactor height.	CHISTI; HALARD; MOO-YOUNG, 1988.
Study of gas retention and liquid circulation in internal circulation airlift reactors containing highly viscous Newtonian and non-Newtonian liquids.	As the viscosity of the liquid increases, the velocity of liquid circulation decreases, and the aeration rate increases.	PHILIP et al., 1990.
Airlift reactor with a net suction tube.	Greater gas-liquid mass transfer is obtained.	WU; WU, 1991.
Airlift reactor with helical flow promoter.	There is the generation of an intense rotational movement of the liquid at the bottom, generating an improvement in the fluidization of the particles.	GLUZ; MERCHUK, 1996.

Airlift reactor with double net draft tubes.	The application of the proposed reactor to the fermentation of Saccharomyces cerevisiae demonstrated that the cultivation time was significantly reduced.	TUNG et al., 1997.
Reator *airlift* de loop interno com tubo de convergência-divergência.	There is a greater gas hold-up in convergence-divergence draft tubes and increases with superficial gas velocity. Variation of structural parameters of convergence-divergence draft tubes has little effect on gas retention in two-phase and three-phase systems.	WEI; XIE; XIAO, 2000.

4 CONCLUSION

Because of the above, one can learn about the Brazilian scenario of biofuels, the operation of an airlift-type bioreactor, the CFD simulation tool, the hydrodynamic parameters that influence the fluid flow in a bioreactor and the studies recorded in the literature on the performance of airlift-type bioreactors.

With this, the objective of making this text a basic research source for those who wish to start studying airlift bioreactors for ethanol production is achieved.

However, carrying out this work should be considered the beginning of research on ethanol production in airlift bioreactors, which can be developed with a more in-depth study of the subject. In new studies on the subject, it is suggested the development of a prototype of the equipment and analysis in CFD

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