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# Hydrodynamic feasibility of the production of biodiesel fuel in a high-pressure reactive distillation column

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ABSTRACT

Among the different processes for producing biodiesel fuel, the use of methanol under conditions near to the critical point is a promissory alternative. The reactive distillation has been proposed to reduce the energy requirements of the esterification step in this process. Such reductions are accompanied by reductions in the total annual costs and the environmental impact. However, due to the conditions under which the column should be operated, special care must be taken in the design of the trays and their hydraulic performance. Proper design of the trays should prevent operational problems. In this work, a strategy for the mechanical design of sieve trays in a homogeneous reactive distillation column is presented. In the column, oleic acid is esterified with methanol under a pressure of 7 MPa. The designs obtained are tested in terms of hydraulics through CFD simulations. CFD analysis is carried out using ANSYS Fluent software.



## Introduction

In recent years, the impact of human activities on the environment has been growing. To meet the global demand for energy, fossil fuels are usually burned; this results in the release of large amounts of greenhouse gases and particles into the atmosphere. In order to reduce the emissions of pollutants, alternative sources of energy have been proposed. Particularly, to satisfy the energy demand in the transport sector, renewable liquid fuels are considered as potential alternatives to fossil fuels, e.g. gasoline and diesel. An alternative is biodiesel, a renewable liquid fuel considered as a potential substitute for petroleum diesel. It has been proved that pure biodiesel has lower emissions of greenhouse gases when burned. Besides, it is non-toxic, has lower sulfur content than fossil diesel, higher cetane number and higher flash point [1–3]. However, pure biodiesel is not used in engines, because it may reduce power and torque [2]. Thus, it is mixed with petroleum diesel for its use as a transport fuel.

There are many different methods for producing biodiesel. One of these methods uses basic and acid homogeneous catalysts [4–6]. The use of heterogeneous catalysts [7–9] and enzymes [10,11] has also been proposed. Other alternatives includes the use of membrane reactors, micro-channel reactors and microwave reactors [12,13].

The use of alcohols under conditions of high temperature and high pressure, close or even higher than the alcohol critical point, has been proposed in recent years [14–16]. Such processes do not require much equipment; however, special materials are required in the construction of the reactor due to the high pressure. Furthermore, the high temperatures proposed for the reaction may cause decomposition of the main product, namely, the biodiesel, and also of the glycerol as by-product [17,18]. Thus, some alternatives have been proposed to reduce the temperature levels required for the reaction, for example, biofuel production in two separate reactors [19]. Supercritical processes are considered an important approach for the production of biofuel, because the yield of the biodiesel thus obtained is not affected by the presence of free

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**Nomenclature**

Symbols used

| | |
|---|---|
| $M_V$ [kg/h] | Mass flow rate for vapor phase |
| $M_L$ [kg/h] | Mass flow rate for liquid phase |
| $A_T$ [m$^2$] | Total area |
| $A_D$ [m$^2$] | Downcomer area |
| $A_N$ [m$^2$] | Net area |
| $A_B$ [m$^2$] | Bubbling area |
| Lw [m] | Weir length |
| Wdc [m] | Downcomer width |
| FPL [m] | Flow-path length |
| S [m] | Tray spacing |
| $d_H$ [cm] | Hole diameter |
| $A_f$ [] | Fractional hole area |
| $h_w$ [cm] | Outlet weir height |
| $h_{cl}$ [cm] | Clearance under the downcomer |
| t [cm] | Tray deck thickness |
| p [cm] | Hole pitch |

fatty acids or water, allowing the use of low-quality raw materials. In this way, a reduction of about 60–80% in the total cost of the process is obtained [20,21]. In order to reduce total energy requirements of the two-step process, the use of reactive distillation to perform the esterification reaction and purification of the products has been recently proposed [22]. It has been found that, even though the reactive distillation column was used only as a pre-purification step (i.e., additional separation is required), this yielded significant reductions in total energy requirements, total annual costs and environmental impact of the production process.

Reactive distillation is an intensified operation in which the reaction and the separation take place in the same equipment, thus reducing equipment costs compared to traditional reactor-separator schemes. Nevertheless, several aspects must be taken into account when designing a reactive distillation column. In the case of heterogeneous reaction, it is important to have an efficient contact of the liquid with the catalyst particles, a good contact between the vapor and the liquid in the reactive zone, a low pressure drop through the catalyst section and sufficient liquid hold-up in the reactive section are aspects that have been reported as very important to the design of catalytic reactive distillation columns [23]. For homogeneous systems, a good liquid distribution, proper vapor/liquid contact and sufficient liquid hold-up are also desired. To obtain high liquid hold-up, Taylor and Krishna [23] proposed the use of modified bubble cap trays.

Computational Fluid Dynamics (CFD) consists in the use of powerful computers and numeric methods for the solution of the transport equations in fluid systems. Its development began in the 60′s and has been used for the analysis of different industrial processes, including distillation columns. Krishna et al. [24] and Van Baten and Krishna [25] described the hydrodynamics in a sieve tray using rectangular and circular geometries and a two-phase transient flow model. The eulerian model was used for both gas and liquid phases, and the liquid height calculated by the simulations was very similar to the experimental data. Van Baten et al. [26] studied the hydrodynamic performance of sieve trays with baffles in a reactive distillation column and reported that the simulation results were similar to the experimental data. Trujillo et al. [27] modelled heat and mass transfer for the evaporation phenomena, concluding that, for such systems, the κ-ε RNG turbulence model represents the experimental data in a better way. Sun et al. [28] reported the use of a κ-ε turbulence model in the simulation of distillation trays with good agreement with the experimental results. Noriler et al. [29] developed a CFD model using an eulerian-eulerian approach to predict the momentum and mass transfer in multiphase flow. Bidimensional, tridimensional and transient models with chemical species, energy and momentum balances were presented in a subsequent work [30]. Rahimi et al. [31] analyzed the effect of the hole size in the efficiency of the tray, using for the analysis an eulerian-eulerian approach. Zarei

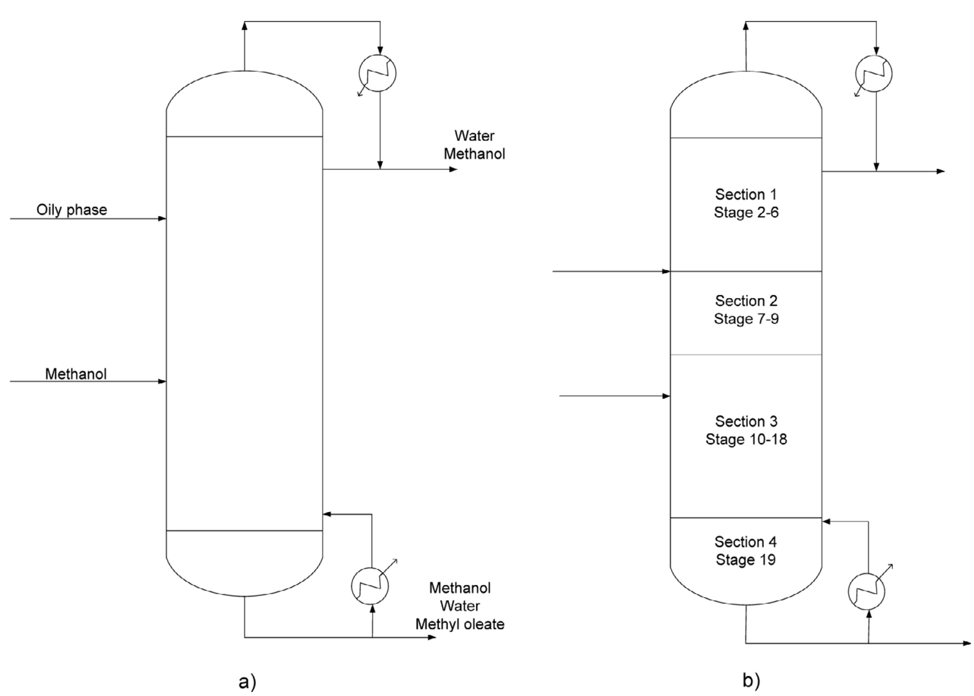


**Fig. 1.** a) Reactive distillation column, b) Distribution of the sections for the mechanical design.