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Numerical simulations of biodiesel synthesis in microchannels with circular obstructions

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ABSTRACT

Biodiesel is considered a viable alternative to the use of diesel. Transesterification is the most used method of biodiesel production and usually occurs in batch reactors and requires several minutes or hours to achieve high yield rates. However, this process has been recently tested in microreactors. One of the most important elements of these microreactors is the micromixer, which should perform a quick and efficient mixing of reactants. Micromixers with circular obstructions split and recombine the flow stream, increasing the interaction of chemical species. Therefore, we carried out numerical simulations of *Jatropha curcas* oil-ethanol mixing and reaction in micromixers with circular obstructions. Three different micromixers were investigated: T-channel, T-channel with circular obstructions and T-channel with alternate circular obstructions. A mixing study was conducted for Reynolds number ranging from 1 to 160 and residence times for reaction of 0.20–100 s. The T-channel with alternate circular obstructions showed the highest degree of mixing (0.99). The presence of obstacles improved the conversion of species. Maximum conversion was 99.07% (T-channel), 99.01% (T-channel with circular obstructions) and 99.09% (T-channel with alternate circular obstructions). The effectiveness of using channels with circular obstructions in biodiesel synthesis was numerically demonstrated.

1. Introduction

Biodiesel is considered a viable alternative to the use of diesel because it has a number of advantages over fossil fuel. It can be manufactured from vegetable oils or animal fats, being a renewable and biodegradable fuel with absence of toxicity, providing many environmental benefits as, reduction of greenhouse gas by 41%, less pollution of air, water and soil, when compared to the use of diesel [1–4].

According to ASTM D6751-15 [5], biodiesel is a fuel that consists of mono-alkyl esters of long chain fatty acids derived from vegetable oils and/or animal fats. Transesterification is the most used method of biodiesel production [1,6]. Transesterification is a class of organic reactions that comprises a transformation of an ester into another through an exchange of acyl groups between esters and acid (acidolysis), esters and other esters (interesterification) or esters and alcohols (alcoholysis) [6]. The variables that can affect the performance of the transesterification reaction are the type and amount of catalyst, the reaction temperature, the molar ratio of alcohol (alcoholysis) and the purity of the reagents [2,4].

The transesterification reaction typically occurs in batch reactors and requires several minutes or hours to achieve high yield [1,7–10]. However, this process has recently been investigated in microreactors, mainly due to the short residence time needed to achieve high conversions [11–14].

Microreactors are generally defined as devices that interconnect microchannels in which small amounts of reagents are handled and reacted for a certain period of time [15]. The advantages of using microreactors rather than batch reactors include: high surface area to volume ratio, enhancing heat transfer, temporal and spatial control of reagents and products and generation of concentration gradients [15,16].

One of the disadvantages of using microreactors in biodiesel synthesis is the difficulty of mixing the reactants, due to the laminar flow. Therefore, the most important elements of these microreactors are the micromixers, which should perform a quick and efficient mixing of reactants. To promote better mixing between vegetable oil and alcohol and increase the efficiency of biodiesel production, several geometries have been proposed, including: reactor with wire coil [17]; T-mixer, J-mixer, rectangular interdigital micromixer and slit interdigital micromixer [18]; Tesla-, Omega-, and T-shaped [19].

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According to the literature consulted by the authors, micromixers with circular obstructions have not been used in the biodiesel synthesis. Geometries with obstructions split and recombine the flow streams, increasing the interactions of chemical species [20]. Fang et al. [21] studied a microchannel with "T" type inlet and a mixing unit with staggered bars, showing its effectiveness for fluid mixing. Alam et al. [22] studied the mixture of water and ethanol in several geometries. Curved micromixers with circular, hexagonal and diamond obstructions were analyzed. Circular and hexagonal obstructions showed similar fluid mixing efficiency, while diamonds present the lowest mixing performance. The circular shape was chosen due to simple geometry and manufacturing convenience.

In the present paper numerical simulations of *Jatropha curcas* oil-ethanol mixing and reaction in micromixers with circular obstructions was carried out. The main goal was evaluate the mixing between these species inside microchannels and predict the best micromixer to study the biodiesel production. Three different micromixers were investigated: T-channel, T-channel with circular obstructions and T-channel with alternate circular obstructions. The micromixer T-channel with alternate circular obstructions was based on Alam et al. [22]. The mixing study was conducted for Reynolds number ranging from 1 to 160 and for the reaction study, residence time was ranged from 0.20–100 s. The *J. curcas* oil was chosen to be a promising source of raw materials, originating from non-edible oil seeds [23] and ethanol that is a biomass derivative, biodegradable and presents low toxicity [2]. It can be highlighted that, considering the published studies with micromixers, this is the first research applying micromixers with circular obstructions for biodiesel synthesis.

2. Micromixers geometry and fluids properties

The micromixers and the identification of dimensions used are shown in Fig. 1. All mixers have the same dimensions and rectangular cross-section. The length of inlet channel (L_e) was 400 μm. The height of mixers (B) was 200 μm. The total mixing length channel (L_m) was 3.51×10^4 μm. The entry length width (W_e) was half the width of the mixing channel (W_m). The widths of the T-channels used were 200, 850 and 1500 μm. For T-channel with circular obstructions and T-channel with alternate circular obstructions the widths were 850 and 1500 μm. For the T-channel with circular obstructions (Fig. 1b), the diameter of obstructions (D_1) was 340 μm for W_m equal to 850 μm and 600 μm for 1500 μm of width of the mixing channel. The distances of obstacles (L_1) were 340 μm (W_m = 850 μm) and 600 μm (W_m = 1500 μm). For the T-channel with alternate circular obstructions (Fig. 1c), the diameters of obstructions (D_2) were 340 μm (W_m = 850 μm) and 600 μm (W_m = 1500 μm). The diameters of the smallest obstacles (D_3) were 255 μm (W_m = 850 μm) and 450 μm (W_m = 1500 μm). The distances between these obstacles (L_2) were 510 μm (W_m = 850 μm) and 900 μm (W_m = 1500 μm).

Geometries and numerical meshes of micromixers was created using ANSYS ICEM 14.0. Tetrahedral elements were used in discretizations. A numerical mesh independence test was performed in a previous study and its parameters were used here [24]. Therefore, the number of control volumes used were 2.98×10^6,

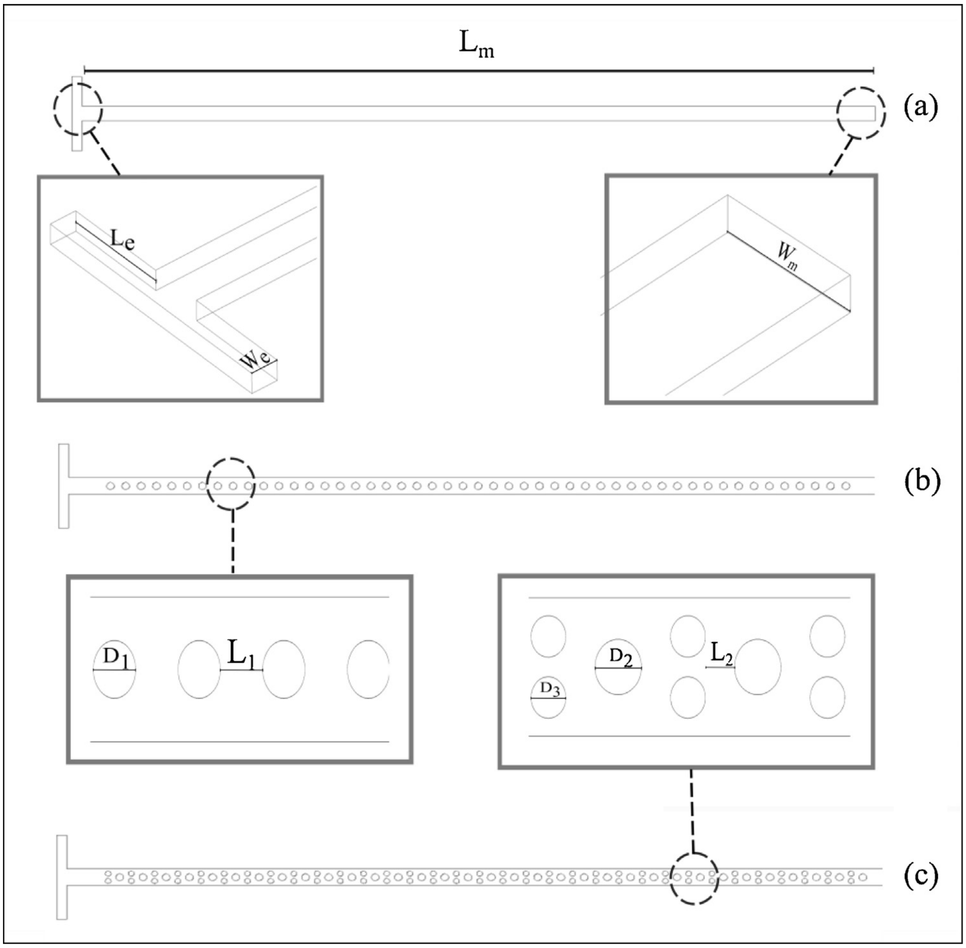

Fig. 1. Micromixers used: (a) T-channel; (b) T-channel with circular obstructions and (c) T-channel with alternate circular obstructions.