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ChemPor 2018

BOOK OF EXTENDED ABSTRACTS

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University of Aveiro & Ordem dos Engenheiros

13th International Chemical and Biological Engineering Conference (CHEMPOR 2018)

Book of Extended Abstracts

Edited by:
João Araújo Pereira Coutinho
Carlos Manuel Silva
Inês Portugal
Ana Barros-Timmons
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SCIENTIFIC PROGRAM

Time		Tuesday, 2/10			Wednesday, 3/10			Thursday, 4/10		
8:00	8:15	Registration								
8:15	8:30									
8:30	8:45									
8:45	9:00									
9:00	9:15				Plenary Lecture (PL3) Rajamani Krishna			Plenary Lecture (PL5) Gabriele Centi		
9:15	9:30									
9:30	9:45	Welcome Session								
9:45	10:00									
10:00	10:15	Plenary Lecture (PL1) Nien-Hwa Linda Wang			O-BB07	O-EE01	O-IM03	O-RS11	O-EE10	O-BS05
10:15	10:30				O-BB08	O-EE02	O-IM04	O-RS12	O-EE11	O-BS06
10:30	10:45				O-BB09	O-EE03	O-IM05	O-RS13	O-EE12	O-BS07
10:45	11:00				O-BB10	O-EE04	O-IM06	O-RS14	O-EE13	O-BS08
11:00	11:15	Coffee-break			O-BB11	O-EE05	O-IM07	O-RS15	O-EE14	O-BS09
11:15	11:30				Coffee-break			Coffee-break		
11:30	11:45	O-RS01	O-BS01	Bondalti						
11:45	12:00	O-RS02	O-BS02	O-MP01	O-BB12	O-EE06	O-ME01	Plenary Lecture (PL6) Nikolaos Hadjichristidis		
12:00	12:15	O-RS03	O-BS03	O-MP02	O-BB13	O-EE07	O-ME02			
12:15	12:30	O-RS04	O-BS04	Prio	O-BB14	O-EE08	O-ME03			
12:30	12:45	O-RS05	O-BB01	O-IM01	O-BB15	O-EE09	O-ME04			
12:45	14:15	Lunch			Lunch			Lunch		
14:15	14:30	Keynotes (KN1 and KN2) João Rocha, Rosa Quinta-Ferreira			Keynotes (KN3 and KN4) Adélio Mendes, José António Teixeira			Keynotes (KN5 and KN6) Maria Ascensão Reis, Ramesh Gardas		
14:30	14:45									
14:45	15:00									
15:00	15:15	O-RS06	O-BB02	BB&G	Plenary Lecture (PL4) María José Cocero			O-RS16	O-EE15	O-IM11
15:15	15:30	O-RS07	O-BB03	O-MP03				O-RS17	O-EE16	O-IM12
15:30	15:45	O-RS08	O-BB04	BP				O-RS18	O-EE17	O-IM13
15:45	16:00	O-RS09	O-BB05	O-MP04				O-MP05	O-IM09	O-IM14
16:00	16:15	O-IM02	O-BB06	O-RS10	Poster Session and Coffee-break P-BB, P-RS, P-MP, P-ME			O-IM08	O-IM10	O-IM15
16:15	16:30	Plenary Lecture (PL2) Paul Christakopoulos						Awards and Closing Session		
16:30	16:45									
16:45	17:00							Multibiorefinery Project Meeting (Coffee-break) CHEMPOR participants are welcome		
17:00	17:15									
17:15	17:30	Formal Session with Minister of Economy								
17:30	17:45									
17:45	18:00				Bus to Vista Alegre Museum Visit					
18:00	18:15	Poster Session and Coffee-break P-BS, P-IM, P-EE								
18:15	18:30									
18:30	18:45									
18:45	19:00									
19:00	19:15									
19:15	19:30									
19:30					Conference Dinner					

[PL] - Plenary Lecture
[KN] - Keynote Presentation
[RS] - Reaction and Separation Processes
[BS]- Biorefinery and Sustainability
[MP] - Modeling, Synthesis and Integration of Chemical Processes

[BB] - Biological Engineering and Biotechnology
[IM] - Innovative Materials and Applications
[EE] - Energy and Environment
[ME] - Multiscale and Multidisciplinary Engineering Education

Biodiesel production through transesterification applying ionic liquids as catalysts

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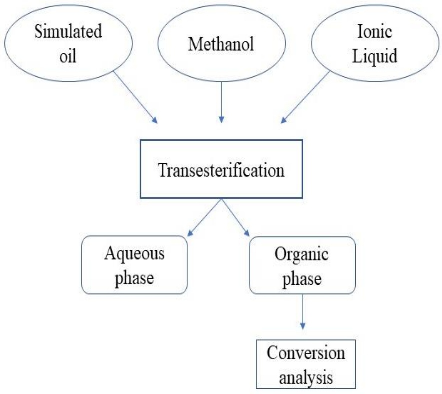

The production of biodiesel started as an alternative and sustainable form of energy to reduce dependence on fossil fuels. This work aims to study the production by transesterification of biodiesel from simulated oil consisting of mixes of waste cooking oil and oleic acid, using as a catalyst ionic liquid (IL) 1-methylimidazolium hydrogen sulfate [HMIM][HSO_4]. The experimental tests were carried out using a two level total factorial design with one replicate, with three parameters: incorporated oleic acid (20% and 40% wt.), molar ratio oil/methanol (1:20 and 1:40) and reaction time (4h and 8h). The fixed operational conditions were: temperature (90ºC) and percentage of catalyst (10% wt.). The response studied was the conversion of the simulated oil. From the statistical analysis of the parameters, it was concluded that the parameters: reaction time and molar ratio oil/methanol, were those that showed the greatest influence on the result.

Introduction

Historically, economic growth was always dependent on energy generation, causing pressure on fossil energy sources. During the 70´s, with a decrease in the supply and an increase in the price of non-renewable fuels, Humanity was faced with the need to involve, in a beneficial way, the economic development and conservation of natural resources, thus seeking alternative and viable forms of energy [1-3].

According to the Brazilian legislation introduced in 2005 [4], biodiesel is a biofuel obtained from renewable biomass for internal combustion engines or energy generation, which can partially or totally replace fossil fuels. Biodiesel is chemically composed of FAME (fatty acid methyl ester), obtained from the chemical reaction of triglycerides with an alcohol, in the presence of a catalyst.

Different raw materials can be used to produce biodiesel, such as used edible vegetable oils (soybean oil, rapeseed oil) or inedible oils (jatropha oil, castor oil), animal fat, waste cooking oils and oil extracted from algae [5].

Acid and basic catalysts are applied to accelerate the reaction rate. For transesterification reaction, basic NaOH or KOH catalysts are the most commonly used. Alternative options for these catalysts are ionic liquids, which are being studied since they enable a more environmentally sustainable biodiesel production process. Among its properties, such substances have potential for recyclability, high catalytic activity, simple operating conditions and high conversion rates for short reaction times [6].

Objectives

The objective of this work is the study of the influence of applying 1-methylimidazolium hydrogen sulfate [HMIM][HSO_4] IL on the catalysis of the transesterification reaction of a highly acidic waste vegetable oil (WVO), in order to assess the viability of the use of acidic imidazolium based IL as catalysts in biodiesel production processes, with further optimization of the main operational conditions: reaction time, reaction temperature, catalyst percentage and oil/methanol molar ratio.

Metodology

Chemicals and raw material. Samples of simulated oils with variable acidity were used as raw material for the transesterification reaction by the incorporation of different contents of oleic acid (90%) in a previously qualitatively and quantitatively characterized WVO. For the reaction, methanol was used. As the catalyst it was used the IL [HMIM[HSO_4].

Transesterification reaction. In the following order, IL, oleic acid, waste cooking oil and methanol were added, in different proportions, to a 100 mL reaction vessel. The vessel was immersed in a paraffin bath, on an automatic heating plate under selected temperature and agitation velocity, coupled with a water reflux condenser. After the reaction time, the mixture was removed from the bath and transferred to centrifuge tubes and stored in the refrigerator for 20h at 4ºC. After this period, the samples were centrifuged at 3000rpm for 20 minutes until the organic and the aqueous phases were completely separated and ready to be splitted. Both phases were stored in vials at 4°C waiting for further analysis.

Experimental design. An experimental design based on a total factorial was generated with three parameters at two levels (2^3) in duplicate: incorporated oleic acid (20% and 40% wt), methanol/simulated oil molar ratio (1:20 and 1:40) and reaction time (4h and 8h). Table 1 describes the 3 parameters chosen, the code applied, and the 2 levels used. The experimental results were analyzed with Design Expert 11 software.

The used methodology defines 16 runs for understanding the influence of each factor on the response. Each run was carried out accordingly to the generic transesterification procedure already presented. One response was evaluated: the conversion of simulated oil, measured according to the procedure described in the European Standard EN14104/2008. The fixed reaction parameters were: temperature, 90°C, and percentage of catalyst, 10% wt.

Table 1. Levels chosen for experimental design.

Parameter	Code	-1	1
Oleic Acid incorporated (%)	A	20	40
Molar ratio oil/methanol (mol/mol)	B	1:20	1:40
Time (h)	C	4	8

Results and Discussion

The factors that influence the conversion of simulated oil were evaluated by using factorial plots: interaction effect and cube plots. ANOVA and p-value significant levels were used to check the significance of the effects on the conversion (R). The experimental results are displayed in Table 2.

Fig. 1 shows the cube plot for the response R (reaction conversion) and the respective levels of oleic acid incorporated (%), molar ratio oil/methanol (mol/mol) and time (h).

The conversion of simulated oil can be expressed using the following equation:

$$R = 88,31 - 1.47A + 4.08B + 4.79C + 0.8410AB + 0.0400AC - 1.16BC \quad (1)$$

This function describes how the experimental variables and their interactions influence the reaction. The model presented an adjusted square correlation coefficient R^2 of 96.7% for the conversion of simulated oil, adjusting the experimental data well.

For the conversion, the reaction time parameter (C) was the most significant, followed by the molar ratio oil/methanol (B), the oleic acid incorporated in the residual oil (A), the BC interaction, the AB interaction and the least significant parameter was the AC interaction. The variables presented the value of p-value, respectively, of 9.45×10^{-8}, 3.74×10^{-7}, 1.10×10^{-3}, 4.90×10^{-3}, 2.48×10^{-2} and 9.01×10^{-1}. It is noteworthy that the lower the value corresponding to p-value bigger is the significance of the parameter for the presented result.

Fig. 2 corresponds to interactions of effects between variables. A significant interaction results when the lines are not parallel. These plots indicated that interaction between molar ratio oil/methanol and time (BC) was stronger than between oleic acid incorporated and molar ratio oil/methanol (AB) and the interaction between oleic acid incorporated and time (AC) was statistically significant but much smaller.

Conclusion

The factor of greatest influence in the conversion was the reaction time, followed by the molar ratio oil/methanol. The factorial experiments showed a significant interaction between the two variables of greater influence. These parameters had a positive influence on the conversion rate studied.

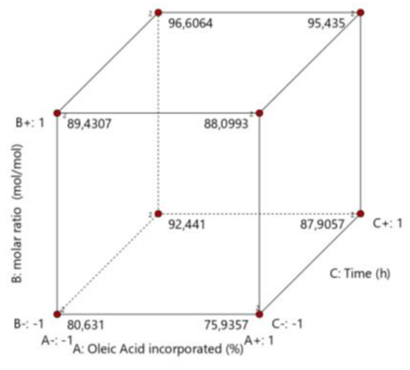

Figure 1. Cube plot for conversion (R).

Table 2. Experimental responses.

Run	Coded values			Responses	
	A	B	C	**R1 (%)**	**R2 (%)**
1	1	1	1	93.96	96.80
2	-1	-1	1	90.85	93.91
3	1	-1	-1	74.89	76.87
4	-1	1	1	96.92	96.41
5	1	-1	1	87.09	88.83
6	-1	-1	-1	79.86	81.51
7	-1	1	-1	89.34	89.41
8	1	1	-1	88.55	87.76

R: Values obtained for the conversion of simulated oil; R1 and R2 correspond to duplicates.

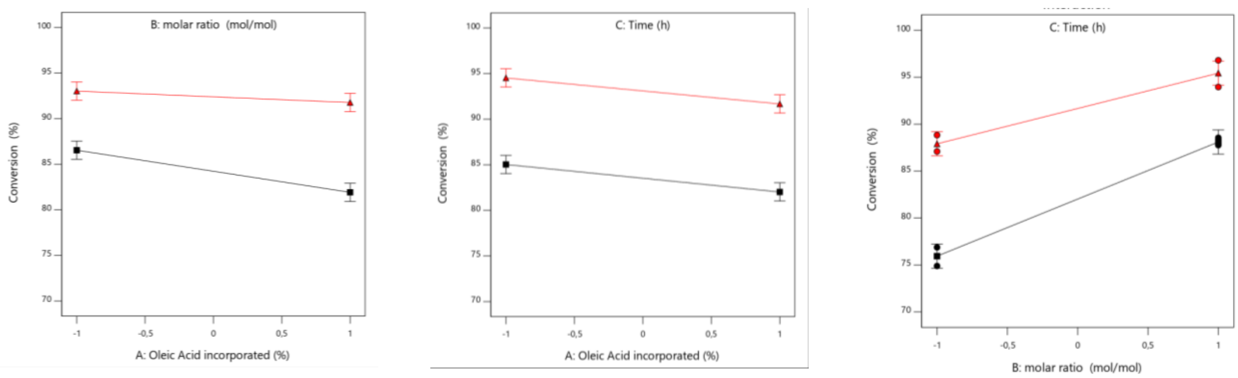

Figure 2. Interaction effects plot for conversion (R).

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