Energy Conversion and Management 160 (2018) 251–261

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

Multi-objective exergy-based optimization of continuous glycerol ketalization to synthesize solketal as a biodiesel additive in subcritical acetone

Mortaza Aghbashlo[a,*], Meisam Tabatabaei[b,c,*], Soleiman Hosseinpour[a,*], Hajar Rastegari[d], Hassan S. Ghaziaskar[d]

[a] Department of Mechanical Engineering of Agricultural Machinery, Faculty of Agricultural Engineering and Technology, College of Agriculture and Natural Resources, University of Tehran, Karaj, Iran
[b] Microbial Biotechnology Department, Agricultural Biotechnology Research Institute of Iran (ABRII), P.O. Box: 31535-1897, Agricultural Research, Education, and Extension Organization (AREEO), Karaj, Iran
[c] Biofuel Research Team (BRTeam), Karaj, Iran
[d] Department of Chemistry, Isfahan University of Technology, Isfahan, Iran

ARTICLE INFO

Keywords:
Adaptive neuro-fuzzy inference system
Biodiesel additive
Exergy analysis
Glycerol conversion
Non-dominated sorting genetic algorithm-II
Solketal synthesis

ABSTRACT

This study was aimed at exergetically investigating and optimizing a continuous reactor applied to valorize glycerol into solketal as a biodiesel additive with subcritical acetone in the presence of Purolite PD206. The effects of reaction temperature (20–100 °C), acetone to glycerol molar ratio (1–5), feed flow rate (0.1–0.5 mL/min), pressure (1–120 bar), and catalyst mass (0.5–2.5 g) were evaluated on the exergetic performance parameters of the reactor. In order to optimize the operating conditions of the reactor, adaptive neuro-fuzzy inference system (ANFIS) was coupled with non-dominated sorting genetic algorithm-II (NSGA-II). The ANFIS was applied to develop objective functions on the basis of the process parameters. The developed objective functions were then fed into the NSGA-II to find the optimum operating conditions of the process by simultaneously maximizing universal and functional exergetic efficiencies and minimizing normalized exergy destruction. Overall, the process parameters significantly affected the exergetic performance of the reactor. The ANFIS approach successfully modeled the objective functions with a correlation coefficient higher than 0.99. The optimal ketalization conditions of glycerol were: reaction temperature = 40.66 °C, acetone to glycerol molar ratio = 4.97, feed flow rate = 0.49 mL/min, pressure = 42.31 bar, and catalyst mass = 0.50 g. These conditions could be applied in pilot- or industrial-scale reactors for converting glycerol into value-added solketal in a resource-efficient, cost-effective, and environmentally-friendly manner.

1. Introduction

Over the last few years, biofuels have drawn an increasing deal of attention as alternatives to fossil fuels due to their environmental benefits and the fact that they are produced from renewable feedstocks [1]. Among the various biofuels commercialized to date, biodiesel has shown a great potential to supplement petrodiesel [2,3]. Consequently, the production of biodiesel has increased substantially since the year 2000 especially to satisfy the stringent emission mandates for diesel engines and to partially meet the increasing global demand for diesel fuel. This in turn has also led to a glycerol surplus as a by-product of biodiesel synthesis, negatively affecting glycerol price dramatically by up to 10-folds [4]. To improve the economic features of biodiesel industry, upgrading glycerol into different value-added chemicals and making use of glycerol-containing waste streams are crucial.

There are already more than 1500 direct applications of glycerol, particularly in cosmetics, pharmaceuticals, and food industries [5]. Nevertheless, there has been intense research interest towards finding methods to upgrade glycerol into more valuable renewable chemicals. For instance, several well-known value-added derivatives of glycerol are esters [6], acetals [7], and ketals [8]. These chemicals can potentially be used as oxygenated fuel additives to improve diesel/biodiesel combustion and emissions. Among these glycerol derivatives, solketal (4-hydroxymethyl-2,2-dimethyl-1,3-dioxolane) produced from glycerol

* Corresponding authors at: Microbial Biotechnology Department, Agricultural Biotechnology Research Institute of Iran (ABRII), P.O. Box: 31535-1897, Agricultural Research, Education, and Extension Organization (AREEO), Karaj, Iran (M. Tabatabaei).
E-mail addresses: maghbashlo@ut.ac.ir (M. Aghbashlo), meisam_tabatabaei@abrii.ac.ir (M. Tabatabaei), shosseinpour@ut.ac.ir (S. Hosseinpour).

https://doi.org/10.1016/j.enconman.2018.01.044
Received 4 November 2017; Received in revised form 3 January 2018; Accepted 19 January 2018
0196-8904/ © 2018 Elsevier Ltd. All rights reserved.

Nomenclature

$\mathbb{A}$	ash percentage (%)
C	catalyst mass (g)
$\mathbb{C}$	carbon percentage (%)
C_p	specific heat capacity (kJ/kg K)
ex	specific chemical exergy (kJ/kg)
$\dot{E}x$	exergy flow rate (kJ/s)
F	feed flow rate (mL/min)
$\mathbb{H}$	hydrogen percentage (%)
M	molar mass (g/mol)
$\dot{m}$	mass flow rate (kg/s)
$\dot{n}$	molar flow rate (mol/s)
$\mathbb{N}$	nitrogen percentage (%)
$\mathbb{O}$	oxygen percentage (%)
P	pressure (bar)
R	universal gas constant (kJ/mol k)
$\mathbb{S}$	sulfur percentage (%)
T	temperature (°C or K)
x	mass fraction (–)
X	acetone to glycerol molar ratio (–)
y	molar fraction (–)
$\dot{W}$	work flow rate (kJ/s)

Greek letters

ψ	universal exergetic efficiency (%)
ϕ	functional exergetic efficiency (%)
Ψ	normalized exergy destruction (–)

Subscripts

0	dead state
AC	acetone
ch	chemical
des	destruction
ET	ethanol
GL	glycerol
in	inflow
i, j	numerator
l	loss
out	outflow
P	product
ph	physical
q	heat transfer
SK	solketal
WT	water

and acetone has attracted more attention recently due to its unique features in improving cold flow properties and flash point temperatures of both diesel and biodiesel as well as their blends [9]. Solketal can also be used as a solvent and plasticizer, suspension agent in pharmaceutical preparations, and anti-freezing agent [10].

Solketal is conventionally produced through ketalization of glycerol with acetone by using strong Brønsted acid catalysts like sulfuric acid, hydrochloric acid, phosphoric acid, and para-toluene sulfonic acid in solvents such as chloroform, ether, or oil [11]. This procedure suffers from some serious drawbacks such as equipment corrosion, effluent disposal, and difficulties in separation of the catalysts from the products which in turn increase the production cost and result in environmental burdens. These issues can be addressed by using heterogeneous acidic catalysts like nafion [12], zeolite [13], Amberlyst [14], silica containing heteropolyacids [15], and montmorillonite [16]. Batch process has been used for solketal synthesis in the above-mentioned studies. However, this mode of production has several major limitations such as long reaction time, high energy consumption, poor yield, and difficulty in scale-up [17]. Therefore, in order to solve these issues, Shirani et al. [18] developed an easy to scale-up continuous system for upgrading glycerol into solketal in the presence of Purolite PD206 as a heterogeneous catalyst. Even though the developed system efficiently synthesized solketal from glycerol, advanced engineering paradigms such as exergy should still be used to assess the productivity and sustainability of such systems.

During the past two decades, there has been an increasing interest in applying exergy analysis for scrutinizing energy and material conversion systems from productivity and sustainability viewpoints [19–21]. Unlike energy analysis which is based on the first law of thermodynamics, exergy analysis accounts for the degradation of the energy quality by irreversible processes [22]. In better words, by using the first and second laws of thermodynamics simultaneously, exergy analysis compensates for the shortcoming of energy analysis in revealing the energy quality loss because of thermodynamic imperfections [23]. Generally, exergy is not quantitatively conserved like energy but it is destroyed due to irreversibilities within a system [24]. The quantity of destroyed exergy is a measure of environmental pollution costs, providing a quantitative comparison of environmental impacts [25]. Hence, the exergy analysis has been widely used in recent years for analyzing and optimizing various glycerol upgrading processes [26–31]. According to these studies, exergy analysis could provide a better understanding of the effect of process parameters on the thermodynamic performance and can aid with the diagnosis of the most effective strategies to improve the process under investigation.

A number of research works have been reported on the production of value-added chemicals from glycerol with their focus on technical aspects and kinetics simulation of the reported processes [18,32,33]. However, to the best of our knowledge, there is no report so far on the exergy analysis of a continuous or even a batch reactor applied for synthesizing chemicals from glycerol. Therefore, solketal production from glycerol using a continuous reactor with subcritical acetone in the presence of Purolite PD206 catalyst was exergetically analyzed in the present study. According to our previous report, this heterogeneous acidic catalyst could effectively upgrade glycerol to solketal [18]. Therefore, the main aim of the present survey was to enhance our understanding of the ketalization step in the developed continuous reactor exergetically. More specifically, the effects of process parameters viz. reaction temperature (20–120 °C), reaction pressure (1–120 bar), acetone to glycerol molar ratio (1–5), feed flow rate (0.1–0.5), and catalyst loading (0.5–2.5 g) on the exergetic performance parameters of the reactor were comprehensively assessed and discussed. Moreover, a multi-objective exergy-based optimization was carried out to find the optimum operating conditions of the reactor using coupled adaptive neuro-fuzzy inference system (ANFIS) and non-dominated sorting genetic algorithm-II (NSGA-II) approaches. The ANFIS approach was used to develop three objective functions, i.e., normalized exergy destruction, universal exergetic efficiency, and functional exergetic efficiency as a function of the process parameters. The developed objective functions were then fed into the NSGA-II algorithm to simultaneously maximize universal and functional exergetic efficiencies and minimize normalized exergy destruction.

2. Materials and methods

2.1. Materials

Glycerol and acetone (both ≥99%) were purchased from Merck Co. (Germany). Solketal (≥97%) for GC calibration was obtained from Sigma-Aldrich Co. (Germany). Absolute ethanol (ET) was supplied by Bidestan Co. (Iran). Toluene (≥99.9%) was also obtained from Merck.

Download English Version:

https://daneshyari.com/en/article/7159002

Download Persian Version:

https://daneshyari.com/article/7159002

Daneshyari.com