Biodiesel Production by Reactive Distillation: Rapeseed Oil Transesterification Case in the Context of German Bioeconomy

Akan Seitzhanov* and Edwin Zondervan

*Bremen University, Germany, *E-mail:* akansei@uni-bremen.de

Abstract

Biodiesel can replace conventional diesel due to its impact in decrease of greenhouse gases (GHGs) and availability of renewable feedstocks in terms of vegetable oil and animal fats. Conventional biodiesel production processes can be replaced by reactive distillation technology for cost-savings. Process systems engineering (PSE) approaches are vital in investigation of the reactive distillation process due to its complexity and impracticability of conducting experiments without involving simulation tools. This work discusses the need for (dynamic) process models and possible application of integrated process and controller design in biodiesel production.

Keywords: Process modeling, Biodiesel, Transesterification, Reactive Distillation, Rapeseed oil

1. Introduction

During the Global Bioeconomy Summit 2015 (GBS 2015) the term "bioeconomy" was defined as follows: "the knowledge-based production and utilization of biological resources, innovative biological processes and principles to sustainably provide goods and services across all economic sectors". [1] Today around 50 countries are developing or already have developed political strategies to assist the development of sustainable bioeconomy. [2] Apart from the lower carbon economy with reduced greenhouse gas emissions and sustainable production, stimulation of bio-based economy enables wise management of natural resources, improved food security, progress in science and creation of new bio-industry businesses. [3,4]

By 2020, the EU's target is to achieve 10% presence of fuels that originate from renewable sources, like biofuels in the transport fuel market of every EU country. They are considered as an important part of the EU's transport strategy and an alternative to conventional fuels that helps to improve supply security and reduce greenhouse gas emissions. [5] Figure 1 shows projections for the growth of the transportation energy mix. Worldwide an increase of approximately 25% of the global transportation-related energy demand is anticipated by 2040. As a result, it is forecasted that the diesel demand might rise up to 30% to meet marine and trucking needs. [6]

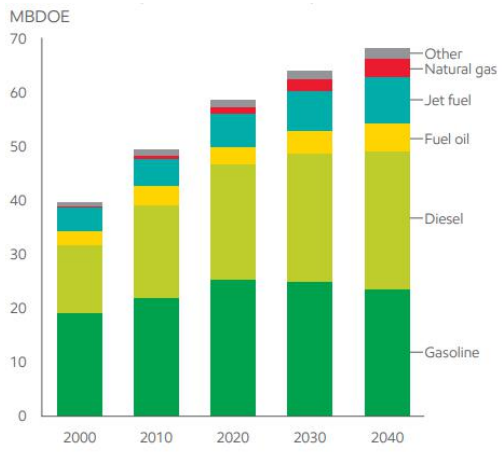

Figure 1: Projections of global transportation energy mix

Nowadays also the maritime transport sector is on the way of reducing CO2 and sulphur emissions. The Marine Environment Protection Committee of the International Maritime Organization (IMO) adopted a legislation controlling the fuels used by ships, allowing to possess not more than 0.5% sulphur content, as of 1 January 2020. [7] Biodiesel is a representative of biofuels that are used as transportation fuels, while biomass being the main feedstock for production. Biodiesel is one of the demanded transportation fuels and global biodiesel production in 2018 was equal to around 34.9 mtoe with Europe accounting approximately 37%. [8] A lower aromatic and sulphur content, a higher cetane number (CN) and a higher biodegradability make biodiesel an attractive fuel over conventional diesel. [9]

Traditionally biodiesel production is performed in a reactor by transesterification reaction between the vegetable oil and a low molecular weight alcohol (e.g., methanol) followed by separators. The reaction products include a complex mixture of fatty acid methyl esters (FAME which is essentially biodiesel) and glycerol as by-product. [10]

However, a promising option is application of reactive distillation for process intensification, reducing energy use, minimizing equipment size, while maximizing productivity. Esterification/Transesterification reaction and the separation of the subsequent products occur in the same unit during the RD. [10] Figure 2 shows how conventional process and reactive distillation process can be compared.[11]

Equilibrium limitations can be overcome by integrating reaction and separation into one unit and this intensifies mass transfer and allows in situ energy integration while simplifying the process flowsheet. This also leads to significant benefits in operating costs and capital investment. [12], [13] In comparison to ordinary distillation, the design of this process is complex due to the strong interactions of chemical reactions and heat and mass transfer. Selection of feed stages (as well as the choice of single and distributed feed), liquid holdup on each tray, catalyst selection are important design parameters that increases the complexity. [14] Complexity of the process makes optimization of process parameters by plainly performing experiments without utilizing simulations impracticable. Hence, modeling and simulation plays key role in achieving optimal design of biodiesel production through RD system and initial development of mathematical model of the RD including reaction and separations zones should be performed prior to simulations studies. [15]

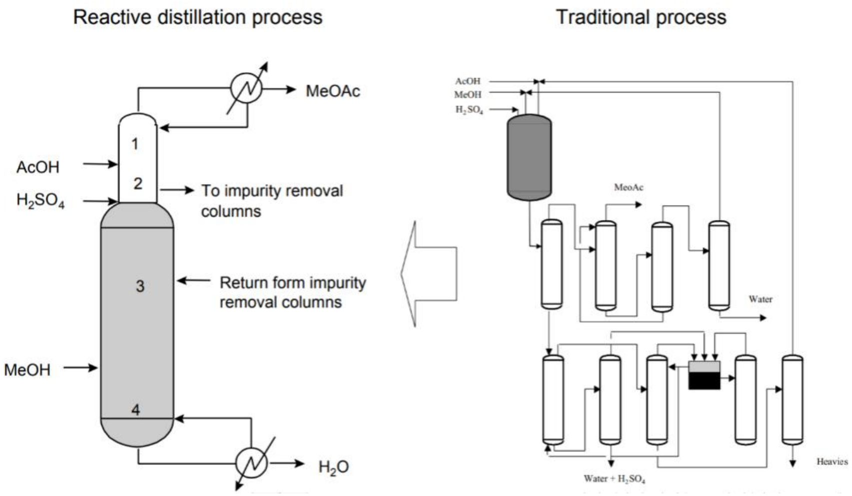

Figure 2: Reactive distillation as process intensification option. Left: reactive distillation setup, right the traditional process.

2. Modeling and simulation of reactive distillation processes

Reactive distillation modeling and simulation have been extensively discussed in the literature. Simasatitkul *et. al*, investigated by simulation the behaviour of transesterification of soybean oil and methanol catalyzed by NaOH in RD column. [16] Poddar simulated two reactive distillation processes for biodiesel manufacturing with heterogeneous and homogeneous catalysts compared the annual production costs, Return-On-Investment (ROI) and payback period. [10] Houge developed models of transesterification of soybean oil with methanol and an optimization of the steady-state model was accomplished using Skogestad's Economic Plantwide Optimisation principles. [17] Agarwal *et. al*, developed a steady-state models for transesterification of oleic esters in the reactive distillation column. In this work the focus was on oil to feed ratio, feed temperature and reaction time. [18]

Rigorous dynamic models of distillation columns entail large numbers of differential and algebraic equations, and to achieve a reduction in equations most of the models are built on simplifications and assumptions. [19] These simplified models with linear tray hydraulics and constant molar flows give substantial deviations from experimental results. [20]

3. Integrated process and controller design

Models are imperative for process design and control. Often design and control models are considered independently: first process design takes place with steady-state economic objectives., while secondly controller design is performed considering process dynamic constraints and operational objectives (such as guaranteeing product quality and operational safety). This sequential approach often associated with issues such as infeasible operating points, process overdesign or under-performance. Thus, by application of this approach a strong performance cannot be achieved every time. [21,22]

In order to achieve optimum economic and control performances controller design needs to be considered in the same time with process design. Simultaneous consideration of process and controller design can be refereed as integrated process design and controller design (IPDC). Identification of variables along with their target values that has importance in process and controller design leads to achieving IDPC. Optimal design values play role of the set-points for the controlled and manipulated variables. [23] According to Abdulhamid [23] IPDC methodologies roughly can be classified and identified as the followings:

A dynamic optimization approach

Based on the way of reformulation of a Mixed Integer Dynamic Optimization (MIDO) problem into a MINLP (Mixed Integer Nonlinear programming) problem it can be classified into simultaneous and sequential methods. For simultaneous strategies all state and control variables are discretized, while in the sequential method which is also known as control vector parameterization, only discretization of control variables occurs. Generally, the dynamic optimization approach can provide an optimal solution but due to the computational complexity it requires huge computational effort, which might lead to difficulties in the context of industrial applications.

An embedded control optimization approach

Embedded control optimization uses a formulation of the IPDC problem as a bi-level optimization problem and it is solved by using two sequential stages to achieve reduction in combinatorial complexity of the initial problem. This approach uses segregation of design and control decisions to maintain manageable size of the problem. Optimal design decisions are looked for in the first stage. At the second stage testing of the dynamic performance which is based on the design decisions (previously obtained) occurs by fixing a particular control along with its tuning parameters. Elimination of integer decisions for selecting controller structures takes place due to the fixing of a particular control strategy in the second stage, and it leads to reduction in problem complexity. Even though this type of approach is quite attractive from the computational point of view and it can be used for solving industrial problems, in some cases suboptimal design solutions are resulted.

A decomposition approach

The general idea of the decomposition approach is formulated in decomposing the optimization problem into set of sub-problems with certain order. Excluding the final subproblem, rest of the subproblems require only the solution of a subset from the original constraints set. The objective function and the remaining constraints form the last subproblem. As a result of this strategy more flexible and relatively simple solution approach can be achieved.

The methods for IPDC clearly show potential for the development of optimal biofuel production via reactive distillation. However, additional inputs should be done for application of IDPC methods for biodiesel production.

4. Conclusions and outlook

Dynamic process models are critical for the development of optimal operational- and design strategies for biofuels production processes. Such comprehensive models can give a precise understanding of the process, while simplified models can deviate from real-life behaviour. In this work we discussed the model development for reactive distillation processes for the conversion of rapeseed oil to biodiesel. We have also discussed about integrating design and control. The IDPS methods should be used for optimal design of biodiesel production via RD.

5. References

Communiqué of the Global Bioeconomy Summit 2015
https://gbs2015.com/fileadmin/gbs2015/Downloads/Communique_final_neu.pdf

Lewandowski I., Bahrs E., Dahmen N., Hirth T., Rausch T., Weidtmann A. (2019). Biobased value chains for a growing bioeconomy. *GCB Bioenergy* 11, 4–8

Bio-based economy in Europe: state of play and future potential - Part 2. (2011).
https://ec.europa.eu/energy/en/topics/renewable-energy/biofuels/overview

McCormick K., Kautto N. (2013). The Bioeconomy in Europe: An Overview. *Sustainability 5*, 2589-2608

European Commission. (2015). Biofuels. https://publications.europa.eu/en/publication-detail/-/publication/af29afb6-105b-47c4- 92ca-38e672262557/language-en

ExxonMobil 2017 Outlook for Energy: A View to 2040.
https://cdn.exxonmobil.com/~/media/global/files/outlook-for-energy/2017/2017-outlook-for-energy.pdf

Cleaner marine shipping with advanced biofuels. (2017).
https://www.upmbiofuels.com/siteassets/documents/other-publications/biofuels-international-march-april-2017-cleaner-marine-shipping-with-advanced-biofuels.pdf

BP Statistical Review of World Energy. (2019). 68th edition.
https://www.bp.com/content/dam/bp/business-sites/en/global/corporate/pdfs/energy-economics/statistical-review/bp-stats-review-2019-full-report.pdf

Haziratul Mardhiah H., Hwai Chyuan Ong, Masjuki H.H., Lim S., Lee H.V. (2017). A review on latest developments and future prospects of heterogeneous catalyst in biodiesel production from non-edible oils. *Renewable and Sustainable Energy Reviews* 67, 1225-1236

Poddar T., Jagannath A., Almansoori A. (2015). Biodiesel Production using Reactive Distillation: A Comparative Simulation Study. *Energy Procedia* 75, 17 – 22

Reactive distillation. Edited by Kai Sundmacher, Achim Kienle. (2002). Wiley – VCH Verlag GmbH & Co. KgaA

Kiss A.A. and Bildea C. S. (2012). A review of biodiesel production by integrated reactive separation technologies. *J Chem Technol Biotechnol* 87,861-879

Kiss A.A., Dimian A. C., Rothenberg G. (2008). Biodiesel by Catalytic Reactive Distillation Powered by Metal Oxides. *Energy Fuels* 22(1), 598-604

Segovia-Hernández J.B., Hernández S., Petriciolet A.B. (2015). Reactive distillation: A review of optimal design using deterministic and stochastic techniques. Chemical Engineering and Processing: Process Intensification 97, 134-143

Kusumaningtyas R.D., Budiman A., Sutijan, Purwono S., Sawitri D.R. (27-30 September 2009). Design of reactive distillation process for a sustainable biodiesel production from palm oil. World Congress on Oils and Fats & 28th ISF Congress, Sydney - Australia

Simasatitkul L., Siricharnsakunchai P., Patcharavorachot Y., Assabumrungrat S., Arpornwichanop A. (2011). Reactive distillation for biodiesel production from soybean oil. Korean Journal of Chemical Engineering 28, 649–655

Houge E. (2013). Reactive Distillation of Biodiesel: Modelling and Optimal Operation. MSc thesis

Agarwal M., Singh K., Chaurasia S.P. (2012). Simulation and sensitivity analysis for biodiesel production in a reactive distillation column. *Polish Journal of Chemical Technology, 14,* ***3,*** *59 —65*

Ingunn Olsen, Guttarm Olav Enrestol and Telje Sira. (1997). "A Rigorous and efficient Distillation Model for engineering and training simulators" Computers chem. Engng, Vol. 21, Suppl., S193-S198

Wittgens, B. and Skogestad, S., (1995). Evaluation of Dynamic Models of Distillation Columns with Emphasis on the Initial Response, IFAC Symposium DYCORD+ '95, Denmark

Seyed Soheil Mansouri, Sales-Cruze M., Huusom J.K., Gani R. (2016) Systematic integrated process design and control of reactive distillation processes involving multi-elements. Chemical Engineering Research and Design, 115, Part B, Pages 348-364

Seyed Soheil Mansouri.(2016). Integrated Process Design, Control and Analysis of Intensified Chemical Processes. PhD thesis, Technical University of Denmark

M. Abdulhamid, Model-Based Integrated Process Design and Controller Design of Chemical Processes, PhD thesis 2011, DTU