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First principle modeling and predictive control of a continuous biodiesel plant

Ana S.R. Brásio [a,b], Andrey Romanenko [b], Natércia C.P. Fernandes [a,*], Lino O. Santos [a]

[a] CIEPQPF, Department of Chemical Engineering, University of Coimbra, 3030-790 Coimbra, Portugal
[b] Ciengis, SA, 3030-199 Coimbra, Portugal

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ABSTRACT

Typically, the large-scale production of biodiesel involves continuous operation plants. Also, the final biodiesel product has to comply with specifications imposed by standards of quality in order to be marketable. These quality constraints must be satisfied during the production at the minimum possible operating cost, in order to make the process economically viable. In this context, a nonlinear model predictive controller (NMPC) is applied to control the oil transesterification section of a continuous biodiesel plant. The controller determines the optimal profiles of the process variables using a nonlinear mechanistic model of the whole transesterification section. The model describes the dynamics of the composition and temperature of the liquid mixture in the reactors and in the decanters, as well as of the decanters interface level. The capability of the proposed NMPC strategy to improve the process economic performance and to enforce the final biodiesel specifications is demonstrated by simulation.

1. Introduction

Biodiesel, an alternative to fossil fuel, has been the subject of a number of research studies covering a wide range of issues, namely oil composition characterization, kinetics of transesterification, alternative uses of the by-product, development of process adaptations to improve its efficiency, and biodiesel and biodiesel blends characterization, just to mention a few. Most of these studies are based on experimental work conducted in laboratory conditions. At an industrial level, the published works related to plant design and optimization are scarcer. Recent reviews on current technologies for biodiesel production and industrial biodiesel practice can be found in [1–5].

The issue of process control in biodiesel plants has also begun to merit more attention. In 2009, Mjalli and Hussain presented a simulation study [6] on the dynamics and control of the biodisel production in a continuous stirred tank reactor where the concentration of ester and the temperature inside the reactor were controlled by manipulating the feed flow rate and the coolant flow rate, respectively. This work was further developed in [7] by using a general control algorithm coupled with a neural network model. In [8], a multivariable adaptative predictive model based control is applied to control the reactor using the recursive least squares algorithm for the ARX model adaptation. In [9], the researchers implemented an adaptive scheme which automatically tunes the internal model controller on the basis of the most recent updated process dynamics and integrates an on-line recursive least squares to model the process. Apart from process design, the work [10] is also devoted to the control of both alkali- and acid-catalyzed processes, with and without glycerol phase recycling. Later, a control system based on programmable logic controller was described in [11] for the batch biodiesel production reaction from waste materials. In 2012, Zhang and co-workers applied plant-wide control concepts to a biodiesel plant [12]. Still in the same year, a model predictive control to track optimal operating conditions of the biodiesel production reaction was proposed in [13], applied to a continuous tubular reactor in which the transesterification occurs under the action of a heterogeneous solid catalyst. The control of an industrial scale batch reactor for biodiesel production was investigated using nonlinear model predictive control technology in [14]. Another contribution [15] approaches the problem of determining the best process configuration and the best controller structure to maximize the profit of a batch biodiesel production plant by using mixed integer nonlinear optimization. Xing et al. applied model predictive control to the biodiesel production process in order to deal with multiple feedstock and low-volume properties, improving the performance of the process [16]. A two-layer predictive control scheme for a continuous transesterification reactor was proposed in [17]. Finally, a plant-wide decentralized feedback control structure was designed and tested for the

* Corresponding author.
E-mail address: natercia@eq.uc.pt (N.C.P. Fernandes).

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Nomenclature

A	heat transfer area of the equipment (m^2)
c_p	specific heat capacity at constant pressure ($J\,kg^{-1}\,{}^{\circ}C^{-1}$)
C	molar concentrations ($mol\,m^{-3}$)
d	vector of disturbances ([d])
E_a	energy of activation ($J\,mol^{-1}$)
F	mass flow rate ($kg\,s^{-1}$)
h	level of the liquid (m)
H_D	height of the liquid inside the decanter ($mol\,m^{-3}$)
k_0	frequency factor (s^{-1})
k	pre-exponential factor of Arrhenius's Law (s^{-1})
m	mass of the liquid (kg)
M	molecular weight ($kg\,mol^{-1}$)
p	predictive horizon (dimensionless)
r	overall reaction rates ($mol\,s^{-1}\,m^{-6}$)
R	ideal gas constant ($J\,mol^{-1}\,{}^{\circ}C^{-1}$)
R_{ao}	alcohol to oil mass ratio (dimensionless)
S	set of input streams to the reactor (dimensionless)
T	temperature of the liquid (°C)
u	vector of manipulated variables ([u])
U	vector of initial predictive control profiles ([U])
U^*	overall heat transfer coefficient ($W\,m^{-2}\,{}^{\circ}C^{-1}$)
V	volume of the liquid (m^3)
x	vector of state variables ([x])
X	vector of initial predictive state profiles ([X])
$\bar{X}$	vector of state predictions ([$\bar{X}$])
y	vector of output variables ([y])
$\bar{Y}$	vector of output predictions ([$\bar{Y}$])
z	control horizon (dimensionless)
α	energy flow to/from the reactor (W)
ΔH_r	heat of reaction ($J\,mol^{-1}$)
θ	vector of parameters ([θ])
λ_v	control valve aperture (%)
ξ	split fraction to the heavy phase (dimensionless)
ρ	mass density ($kg\,m^{-3}$)
ϕ	generation reaction term ($mol\,s^{-1}$)
Ψ	objective function (dimensionless)
χ	final mass fraction (% (m/m))

Subscripts

0	inlet stream
a	alcohol
air	air
D	decanter
H	heavy phase of the decanter
L	light phase of the decanter
o	oil
R	reactor
r	reaction

Acronyms

D	decanter
E	esters of fatty acids
G	glycerol
M	methanol
R	reactor
DG	diglyceride
MG	monoglyceride
TG	triglyceride
PID	proportional-integral-derivative
UKF	unscented Kalman filter
NMPC	nonlinear model predictive control

continuous manufacture process of biodiesel using a sugar catalyst. The control problem of plants with more specific designs (using equipment such as a biodiesel microwave reactor or reactive absorption columns) has also been studied in [18–20].

Model predictive control has been applied with success in large scale processes, such as refineries and petrochemical plants where it delivers sustainable economic results. However, this technology is applicable to smaller scale processes, as well [21]. Biodiesel plants seem to have great potential for advanced control. Indeed, the final product has to comply with the stringent quality standards, one of the reactants is used in excess and must be recovered with an energy intensive process (distillation), the reaction depends on operating conditions in a nonlinear way and the raw material may exhibit high variability. This work discusses the application of a nonlinear, first principle based model predictive controller to the operation of oil transesterification in a continuous biodiesel plant and expands the previous publication [22] where some preliminary results were shown. The main motivation of this application is to improve the economic performance of the production process while complying with the demanding quality standards. This is achieved by pushing the key quality variables closer to the bounds in the direction of the economic optimum.

It is shown that complementing a regulatory layer made of PID controllers with the advanced control technique yields tangible economic results as it takes into account the process variables interactions and their nonlinearity in a predictive way. For instance, in the oil transesterification section, a change in the production causes not only an adjustment of the total flow rate of chemicals (methanol) but also its different distribution among the reaction vessels. The performance of the approach is demonstrated by simulation in disturbance rejection and servo control scenarios.

This work leverages these positive traits of NMPC and shows that the corresponding benefits may be obtained at production sites such as biodiesel plants, where NMPC is not yet a common practice. The multivariable, plantwide approach minimizes the consumption of reactants and utilities and ensures the operation within pre-defined bounds of a large biodiesel plant of Lurgi design. To the best of authors knowledge, such application has not been reported in the literature until now. A description of the biodiesel plant oil transesterification section is presented in Section 2, along with the dynamic model formulation, the methods for the calculation of the thermo-physical properties, and the definition of the biodiesel quality indicators. The NMPC formulation and control problem statement are described in Section 3. Simulation results that show the advantages of using NMPC as a complementary advanced control technology for economic and operation performance are presented in Section 4. Finally, concluding remarks are given in Section 5.

2. Biodiesel plant

A simplified piping & instrumentation diagram of a continuous biodiesel plant, based on the Lurgi design, is sketched in Fig. 1. The plant features two continuous stirred tank reactors (R1 and R2) in series, each with a capacity of 14.0 m^3, and two decanters (D1 and D2) of 4.7 m^3 each. The typical production rate scenario considered in this study is one of an average vegetable oil feed rate that can vary between 120 and 240 t/d. The vegetable oil feed of reactor R1 is pre-heated up to a desired temperature to favor the transesterification reaction of the triglycerides with methanol to form the raw ester. The reactors are fed with the required flow rates of alcohol (methanol) and of catalyst (KOH) alcohol solution. The reactor mixture is sent to decanter D1 where a separation between light and heavy phases occurs. The light phase, rich in ester, is fed to reactor R2. The outlet flow rate of reactor R2 is sent to decanter D2. Here, the