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SENSITIVITY ANALYSIS AND MULTIOBJECTIVE OPTIMIZATION OF DIFFERENT BIODIESEL PRODUCTION PROCESSES

G. Di Nicola¹, M. Moglie¹, G. Santori²

¹*Università Politecnica delle Marche, Facoltà di Ingegneria, Dipartimento di Energetica, Via Brecce Bianche, Monte Dago, 60131 Ancona, Italia*

²*The University of Edinburgh, School of Engineering, Institute for Materials and Processes, Sanderson Building, The King's Buildings, Mayfield Road, EH9 3JL, Edinburgh, Scotland, UK*

ABSTRACT

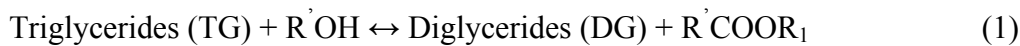
One of the most promising renewable fuels proposed as an alternative to fossil fuels is biodiesel. The competitive potential of biodiesel is limited by the price of vegetable oils, which strongly influences the final price of biofuels, but an appropriate planning and design of the whole production process, from the seed to the biodiesel end product is essential to contain the fallout of energy inefficiencies in the high price of the end product. This study focuses on the characteristics of the production process currently used to produce biodiesel.

The refined vegetable oil can be converted into biodiesel by means of a great variety of techniques and technologies, many of which are still not suitable for applications on industrial scale. The solution that has the greatest interest is homogeneous alkaline transesterification with KOH and methanol. Even when we dealing with this type of conversion, it is impossible to establish a universal pattern to describe the conversion or purification stages because there are various possible solutions that make every systems different from each other. When we then look more closely at the state of the art in industrial biodiesel production plants, we encounter the potential problems introduced by the type and characteristics of the raw materials.

Comparing some of the reference solutions that have inspired numerous installations, a statistical sensitivity analysis is conducted using ASPENPLUS[®], after the identification of the main parameters in each process. The statistical sensitivity analysis has been carried out by a multi-objective genetic algorithm optimization, to define the configurations of the main parameters that guarantee the best trade off between the maximization of some important compound purity and minimization of energy requirements in the process. The results of this analysis was a Pareto frontier that identifies a family of configurations that define the best trade off between the objectives. From the Pareto frontiers we have then selected the configuration that require the minimum consumption of energy. There is between these optimal configurations a configuration which require a specific energy consumption, for PROCESS-I of 2.7 MJ/kg and 1.5 MJ/kg for PROCESS-II. The biodiesel obtained from these two different layout, dealing with the requirements given by the UNI EN 14214, the methanol recycled has a purity higher than 97% by weight and glycerol a purity higher than 90 %.

INTRODUCTION

Biodiesel is a mixture of fatty acid methyl esters derived from the triglycerides contained in vegetable oils (Meher et al., 2006). There are various methods for converting vegetable oils into biodiesel, but the most often used is a transesterification reaction between an alcohol and the vegetable oils, induced by a catalyst to form fatty acid methyl esters and glycerol (Ma and Hanna, 1999). The nature of the transesterification reaction depends on the type of catalyst used, which may be alkaline, acid or enzymatic. Transesterification is a three-step reaction in which triglycerides are converted consecutively into diglycerides, monoglycerides and glycerol, fatty acid methyl esters being produced in each step (Marchetti et al, 2007).



Alkaline transesterification is more efficient and takes place faster than its acid counterpart, but the oil being treated should be anhydrous and have an acid value below 1 (Wright et al., 1944). Any water in the reacting mixture will use up the catalyst, reducing the yield from the reaction.

Designing the industrial biodiesel production process involves considering all the stages of conversion and biodiesel purification, and the equipment required. Here, we consider two possible industrial processes, based on the alkaline transesterification of refined vegetable oil. The processes were modeled with ASPENPLUS[®], for a transesterification reaction with KOH and methanol at a temperature of 60°C. Then we studied the problem of optimization, considering the specific energy consumption to produce biodiesel with the standards required by the UNI EN 14214. The optimization problem was solved using multiobjective genetic algorithm.

PROCESS DESIGN

To optimize the process and identify the configuration with the lowest specific energy consumption, complete process simulations were performed with the ASPENPLUS[®] software. The software includes a full database of compounds to choose from. The compounds needed are methanol, KOH, glycerol, potassium phosphate, phosphoric acid, water, triolein, and methyl oleate. The software require the determination of the proper thermodynamic model, to predict the phase equilibria of the systems. The thermodynamic models proposed in literature, for biodiesel mixture, are numerous. The most suitable are the GCA-EOS and the A-UNIFAC (Andreatta et al., 2007). Good prediction is also assured by the UNIFAC-DORTMUND model, that is present in ASPENPLUS[®] (West et al., 2008).

For the simulation we also needed to identify the layout of the process, defining all the equipment required and their relative position. The two processes considered are illustrated in Figs 1-2. The processes analyzed here treated about

2000 kg/h of sunflower oil, using an oil to methanol ratio of 1:6 and a KOH ratio of 1% by mass of vegetable oil.

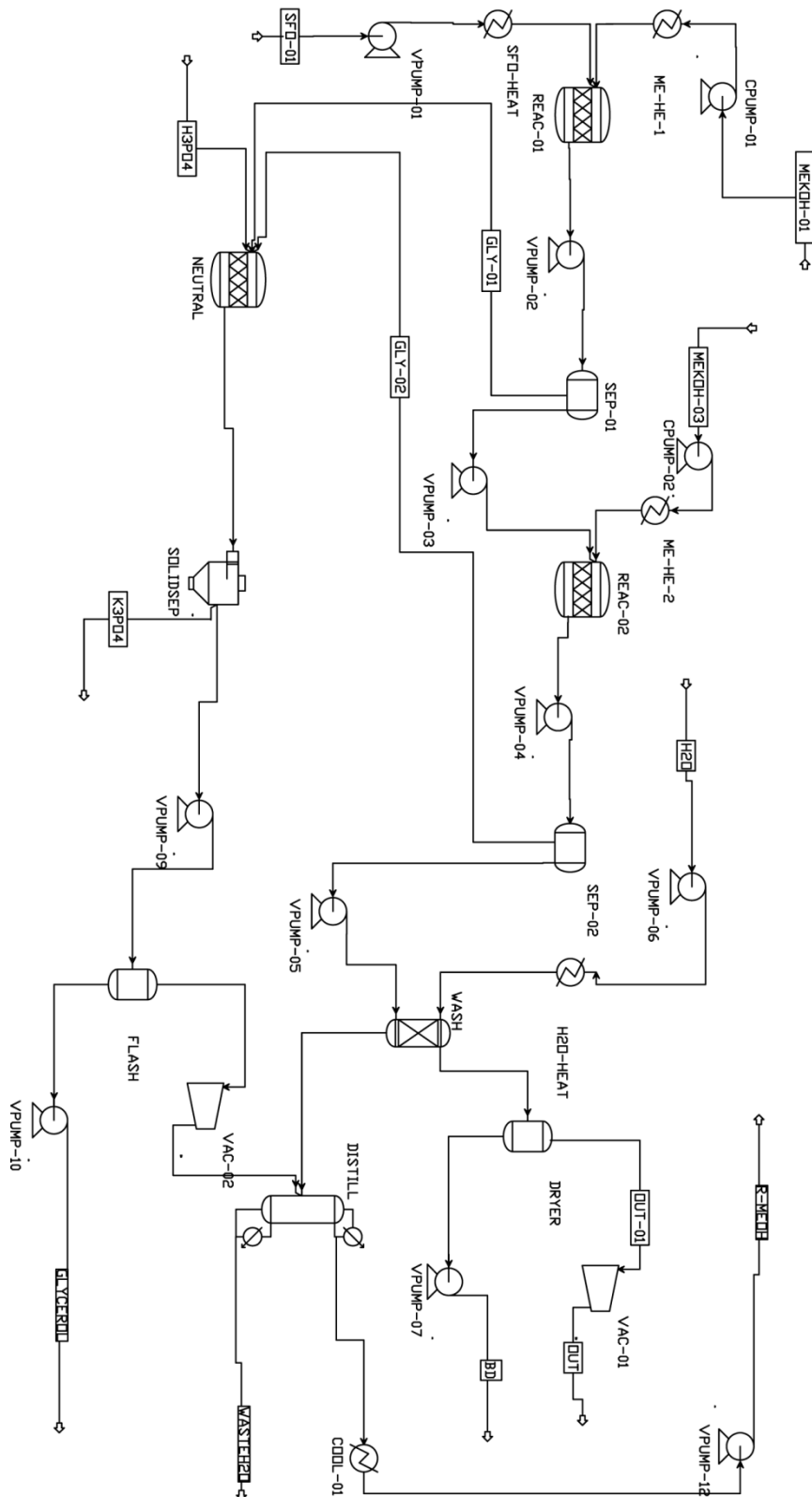


Figure 1 PROCESS-I layout

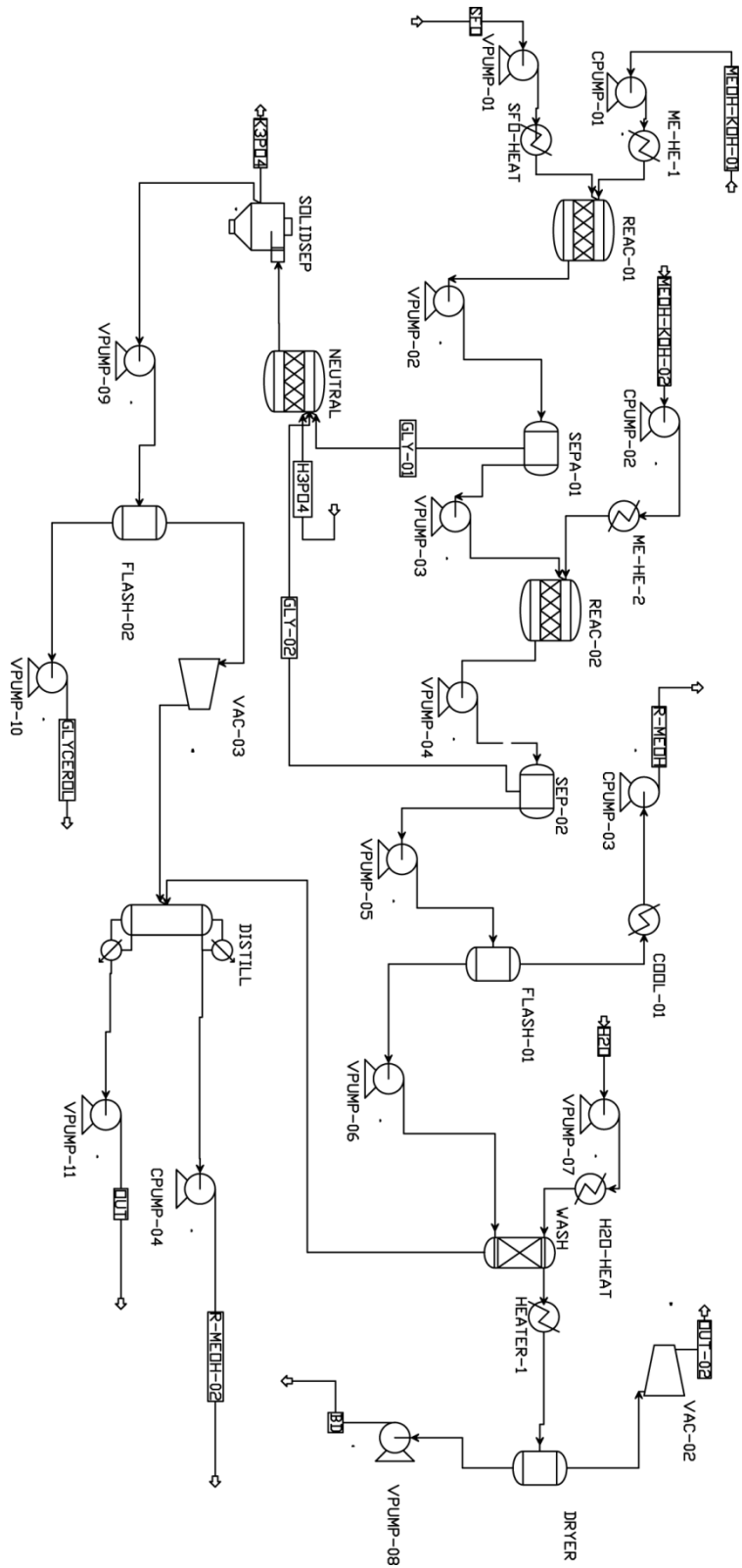


Figure 2 PROCESS-II layout

PROCESS OPTIMIZATION

The optimization of an entire process, is a difficult task. The problem require the identification of all variables, objectives and constraints to be met. Multi-objective optimization identifies a set of optimal trade-offs that can satisfy all the constraints and objectives defined (Abraham et al., 2005). The result of the optimization procedure is a Pareto-optimality, from which to choose the solution of the problem of optimization.

Optimization was done with the modeFRONTIER™ software, which is a tool that facilitates the analysis of optimization problems. The software require the definition of the variables, constraints and objectives, and the optimization algorithm to be used. Two different objective function have been defined, one that represents the quality of compounds produced and one relative energy consumption. These two functions are has follow:

$$Y = \frac{\dot{m}_{BD} * x_{BD} + \dot{m}_{GLY} * x_{GLY} + \dot{m}_{MEOH} * x_{MEOH}}{\dot{m}_{BD} + \dot{m}_{GLY} + \dot{m}_{MEOH}} \quad (4)$$

$$Z = E_T \quad (5)$$

The constraints defined are that ruled by UNI EN 14214, for biodiesel, and purity for glycerol and methanol produced.

The optimization algorithm used is the multi-objective genetic algorithm. This algorithm use an elitism operator able to preserve some excellent solutions without bringing premature convergence to local-optimal frontiers (Abraham et al., 2005). The algorithm require the identification of a space of solutions, from which starting the generations. The starting domain is that defined by full factorial design algorithm.

PROCESS-I consisted of a two-step reactor with an intermediate decanter (SEP-01) for separating the glycerol from the biodiesel. The output from the second decanter (SEP-02) was delivered to a liquid-liquid extraction column (WASH), where water was used as the solvent to remove any residual glycerol and unreacted methanol from the biodiesel. After this treatment, the biodiesel was sent to a dryer (DRYER) to eliminate any residual water and thus comply with the UNI EN 14214. The separated glycerol was delivered to a neutralizing reactor (NEUTRAL), where the residual catalyst was removed. After neutralization, the methanol was extracted by a flash distillation unit (FLASH-01) and the glycerol obtained was delivered to a storage tank. The methanol extracted from the glycerol stream and the waste water from the liquid-liquid extraction column was sent to a distiller column (DISTILL), which is needed to further purify the methanol and enable its recovery and reuse. In PROCESS-II indeed, once the glycerol has been separated from the biodiesel, the unreacted methanol was extracted from the reaction mixture by means of a flash distillation unit (FLASH-01), and the biodiesel was treated in a liquid-liquid extraction column. To comply with legal requirements, the biodiesel was then dried (DRYER). The separated glycerol was delivered, after neutralizing (NEUTRAL) the catalyst, to a flash distilling unit (FLASH-02). The methanol extracted and the waste water were delivered to a distilling column (DISTILL) to ensure the maximum methanol quality and the minimum methanol content in the waste water. The variables and their range of

variability, for each processes are listed in table 1.

Table 1 Processes variables and range of variability

PROCESS-I				
		Lower Value	Intermediate Value	Upper Value
T_{Water}	[°C]	30	65	100
Reflux Ratio		0.8	2.9	5
N_{Stage}		10	20	30
T_{Flash}	[°C]	90	145	200
T_{Dryer}	[°C]	120	185	250
\dot{m}_{Water}	[kg/h]	70	185	300
PROCESS-II				
		Lower Value	Intermediate Value	Upper Value
T_{Water}	[°C]	30	65	100
Reflux Ratio		0.75	1.12	1.5
$T_{\text{Flash-01}}$	[°C]	75	112	150
$T_{\text{Flash-02}}$	[°C]	75	112	150
T_{Dryer}	[°C]	120	185	250
\dot{m}_{Water}	[kg/h]	100	400	700

The outcome of optimization is a set of solutions representing the Pareto frontier, which is given in figure 3 for PROCESS-I and in figure 4 for PROCESS-II. The Pareto frontier obtained represents the energy requirements for a given process configuration.

RESULTS AND DISCUSSION

The Pareto charts obtained, plot the energy requirements against the quality of the material produced for each configurations. To identify which is the process with the smallest amount of energy consumed, a specific energy consumption was calculated. The specific energy consumption is obtained dividing the energy consumption by the flow rate of biodiesel output for each process.

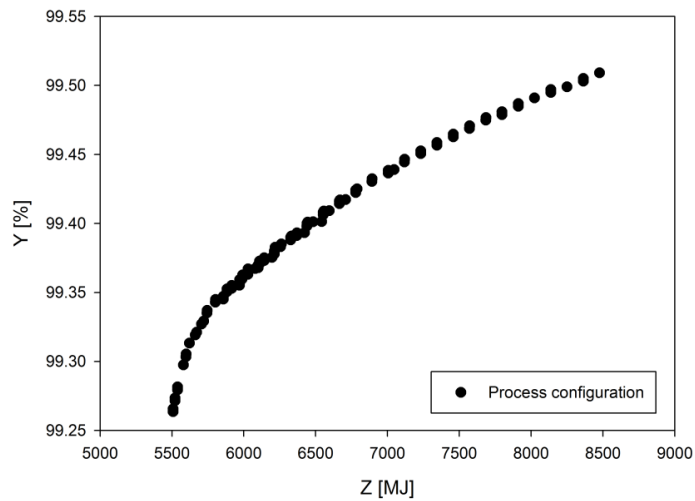


Figure 3 PROCESS-I Pareto Frontier

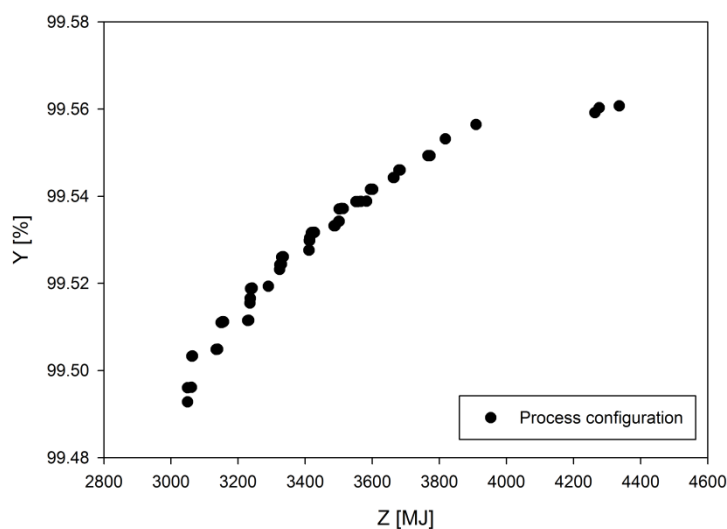


Figure 4 PROCESS-II Pareto Frontier

The configuration used for each process, is that identified by the intersection of the minimum energy consumed and minimum quality of material produced. The configurations identified and the technical results obtained are shown in table 2.

Table 2 Process configurations and technical results

PROCESS-I			PROCESS-II		
T_{Water}	[°C]	36	T_{Water}	[°C]	32.5
Reflux Ratio		2.8	Reflux Ratio		0.84
N_{Stage}		17	$T_{\text{Flash-01}}$	[°C]	75.5
T_{Flash}	[°C]	90	$T_{\text{Flash-02}}$	[°C]	148
T_{Dryer}	[°C]	199	T_{Dryer}	[°C]	250
\dot{m}_{Water}	[kg/h]	70	\dot{m}_{Water}	[kg/h]	114

Stream	Flow rate [kg/h]	Purity [%]	Stream	Flow rate [kg/h]	Purity [%]
Biodiesel	1987	99.5	Biodiesel	1984	99.4
Glycerol	246	95.4	Glycerol	216.6	97.7
Methanol	500	98	Methanol	515.3	99.4

Energy consumption	Total [MJ/h]	Specific [MJ/kg]	Energy consumption	Total [MJ/h]	Specific [MJ/kg]
E_T	5507	2.77	E_T	3049	1.53

CONCLUSION

In this work we have compared and optimized two possible processes for the production of biodiesel. The processes has been previously defined in ASPENPLUS[®], defining the flow sheet and the equipments needed and next optimized using modeFRONTIER[™]. The results of the optimization is a Pareto

frontiers, that represents all the possible configurations that represents the best trade-off between energy consumption minimization and material quality maximization. These optimal configurations require a specific energy consumption, for PROCESS-I of 2.7 MJ/kg and 1.5 MJ/kg for PROCESS-II. The quality of biodiesel produced satisfy the standards required for each layout. According with the Pareto frontier the process with the lowest specific consumption is PROCESS-II.

NOTATION

m	mass flow rate, kg/h
x	material purity, %
Y	objective function, %
Z	objective function, MJ
E	energy, MJ
N	number
T	Temperature

Subscripts

BD	biodiesel
GLY	glycerol
MEOH	methanol
T	thermal
Stage	distillation column tray

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