Aspen Plus

Aspen Plus Biodiesel Model

Version Number: V7.0
July 2008

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1 Introduction

This example is a model of a process for the alkali catalysed production of biodiesel from vegetable oil. It is intended to:

- Provide an example of how to model the different areas of this process
- Supply a starting set of components and physical property parameters for modeling processes of this type

The model is not intended for equipment design or for specifying other engineering documents without further review by a process engineer with experience of biodiesel processes.

The model includes:

- A nominal set of chemical species and property parameters for this process.
- Typical process areas including: transesterification, methanol recovery, water washing, FAME purification, catalyst removal, glycerol purification, feed stock recovery and the main streams connecting these units.
- Key process control specifications such as pure methanol flow rate, phosphoric acid flow rate, and specifications for distillation columns.

This model is based upon information included in the following paper:

Y. Zhang, M.A. Dube, D.D. McLean, M. Kates, "Biodiesel Production from waste cooking oil: 1. Process design and technological assessment", *Bioresource Techchnology*, 89:1-16, 2003.

2 Components

The following components represent the chemical species present in the process:

Table 1. Components Used in the Biodiesel Model

ID	Type	Formula	Name
METHANOL	CONV	METHANOL	CH4O
OIL	CONV	TRIOLEIN	C57H104O6
FAME	CONV	METHYL-OLEATE	C19H36O2
GLYCEROL	CONV	GLYCEROL	C3H8O3
NAOH	CONV	WATER	H2O
WATER	CONV	WATER	H2O
H3PO4	CONV	WATER	H2O
NA3PO4	CONV	WATER	H2O

Vegetable oil is mixture of several oils and fats. For this example we assume the oil is pure triolein.

FAME, Methyl-Oleate, is the biodiesel product , with glycerol as a by-product.

Sodium hydroxide is used as the catalyst, and is removed adding H_3PO_4 to precipitate Na_3PO_4. Because reaction kinetics and electrolyte chemistry are not modeled in details these electrolytes are modeled using physical property data for water, but with their correct molecular weights.

3 Process Description

This biodiesel process model includes the following units:

Table 2. General Unit Operations Used in the Bio-Diesel Process

Unit	Purpose
Transesterification	Oil reacts with alcohol in the presence of catalyst to yield biodiesel and glycerol
Methanol Recovery	Recover excess methanol
Water Washing	Separate FAME from glycerol and electrolytes
FAME Purification	Purify FAME and recover oil
Catalyst Removal	Remove excess catalyst
Glycerol Purification	Purify glycerol

4 Physical Properties

The models used to calculate physical properties in Aspen Plus are grouped into property methods named after the central model, for example, Ideal, Redlich-Kwong-Soave, and NRTL (Non-Random Two Liquid). The property method used in this model is Dortmund modified UNIFAC. This is suitable for preliminary work. NRTL would probably give more accurate results, but requires estimation of NRTL binary interaction parameters.

5 Chemical Reactions

The reactions modeled are:

Transesterification

OIL + 3 METHANOL $\longrightarrow$ 3 FAME + GLYCEROL   95% conversion of OIL

Catalyst Removal

3 NAOH + H3PO4 $\longrightarrow$ NA3PO4 + 3 WATER   100% conversion of NAOH

This model assumes fixed fractional conversions for each reaction. A more detailed model could model the reaction kinetics. This would require fitting of kinetic parameters to experimental data.

6 Simulation Approach

Unit Operations - Major unit operations in this model have been represented by Aspen Plus blocks as shown in Table 3.

Table 3. Aspen Plus Unit Operation Blocks Used in the Biodiesel Model

Unit Operation	ASPEN-PLUS "Block"	Comments / Specifications
Transesterification	RStoic	Simplified simulation with stoichiometric reactions
Methanol Recovery	RadFrac	Rigorous multi-stage distillation model. 7 theoretical stages.
Water Washing	Liquid-Liquid Extractor	Rigorous multi-stage liquid-liquid extractor model. 6 theoretical stages
FAME Purification	RadFrac	Rigorous multi-stage distillation model. 6 theoretical stages.
Catalyst Removal	RStoic	Simplified simulation with stoichiometric reactions
	Sep	Simplified simulation for solid removal
Glycerol Purification	RadFrac	Rigorous multi-stage distillation model. 6 theoretical stages.

Streams - Streams represent the material and energy flows in and out of the process. Streams can be of three types: Material, Heat, and Work. Feeds to the biodiesel model are oil, methanol, sodium hydroxide, water and acid.

Design-Specs, Calculator Blocks - The simulation includes a Design Spec and Calculator Block as shown in Tables 4 & 5:

Table 4. Design Specs Used in the Biodiesel Model

Spec Name	Spec (Target)	Manipulated Variable
MEOHCONC	Mass fraction of methanol in reactor outlet is 0.092	Methanol feed stream flow rate

Table 5. Flowsheet Calculators Used in the Biodiesel Model

Name	Purpose
PO3FLOW	H_3PO_4 feed flow is determined according to excess sodium hydroxide

7 Simulation Results

The Aspen Plus simulation flowsheet is shown in Figure 1.

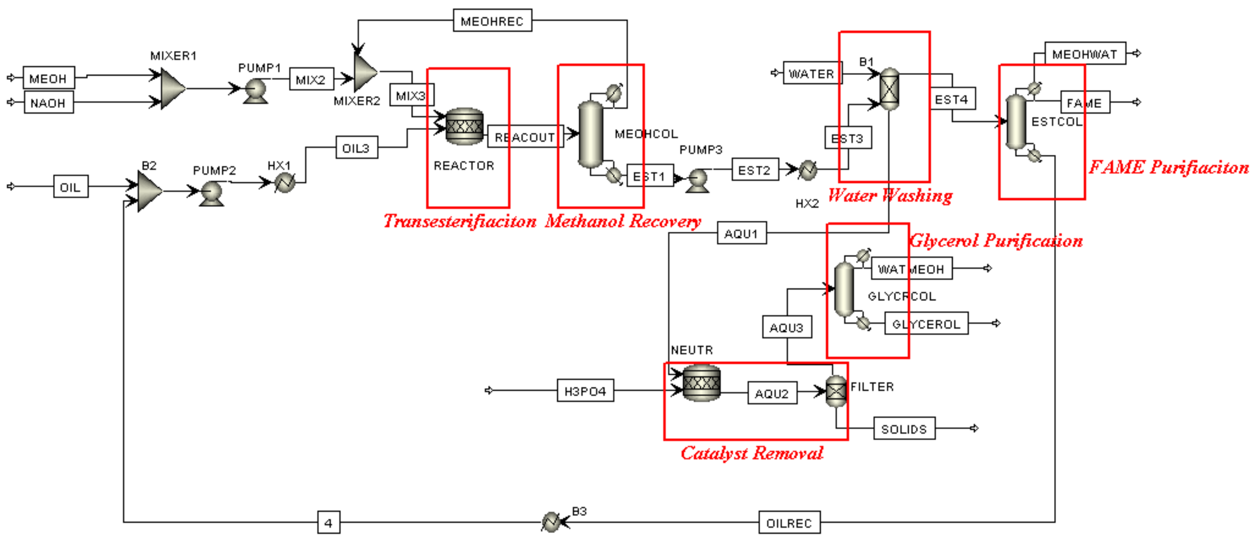

Figure 1. Biodiesel Flowsheet in Aspen Plus

Key simulation results are presented in Table 6.

Table 6. Key Simulation Results

Plant capacity (pure FAME)	9.23	MM kg/yr
Oil feed	1050	kg/hr
Methanol feed	121.418	kg/hr
Catalyst feed	50	kg/hr
H3PO4 feed	40.8	kg/hr
Water feed for washing	50	kg/hr
Transesterification reactor biodiesel composition	0.753	Mass fraction
Product FAME purity	0.997	Mass fraction
Product Glycerol purity	1	Mass fraction

8 Conclusion

The Biodiesel model provides a useful description of the process. The model can be used as a guide for understanding the process and the economics, and also as a starting point for more sophisticated models for plant design and specifying process equipment.