Chapter 7
Optimization of Industrial Process 2

This example analyzes the production of biodiesel from degummed soybean oil. The included SuperPro Designer® model is a slightly modified version of a process model developed by Haas et al. (2006).

There has been intense investigation on the development of fuel producing processes that are based on the use of renewable agricultural materials as feedstock. This activity is driven by the quest of national fuel self-reliance as well as reducing emissions of particulates, hydrocarbons, and carbon monoxide. Most of efforts have been concentrated on bioethanol and biodiesel. Biodiesel consists of the simple alkyl esters of the fatty acids found in agricultural acylglycerol-based fats and oils. It has been shown to give engine performance similar to that of conventional fuels.

Biodiesel can be produced from any material that contains fatty acids. Thus, various vegetable fats and oils or animal fats can be used as feedstocks for the biodiesel process. The choice depends on local availability, cost, and government regulations.

Here are the three most dominant ways of biodiesel production:

- Base-catalyzed transesterification of the oil
- Direct acid-catalyzed transesterification of the oil
- Conversion of the oil to its fatty acids and then to biodiesel

Most of the biodiesel produced today is done with the base-catalyzed reaction for several reasons:

- It requires low temperature and pressure.
- It yields high conversion (98%) with minimal side reactions and reaction time.
- It is a direct conversion to biodiesel with no intermediate compounds.
- No need for exotic materials of construction.

The chemical reaction for base-catalyzed biodiesel production is depicted below (Fig. 7.1).
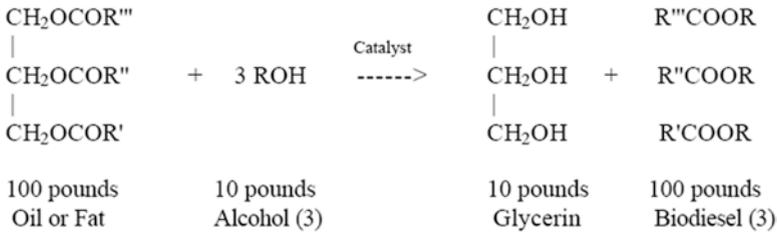
The Biodiesel Reaction

CH₂OCOR‴			CH₂OH		R‴COOR
CH₂OCOR″	+ 3 ROH	$\xrightarrow{\text{Catalyst}}$	CH₂OH	+	R″COOR
CH₂OCOR′			CH₂OH		R′COOR

100 pounds	10 pounds	10 pounds	100 pounds
Oil or Fat	Alcohol (3)	Glycerin	Biodiesel (3)

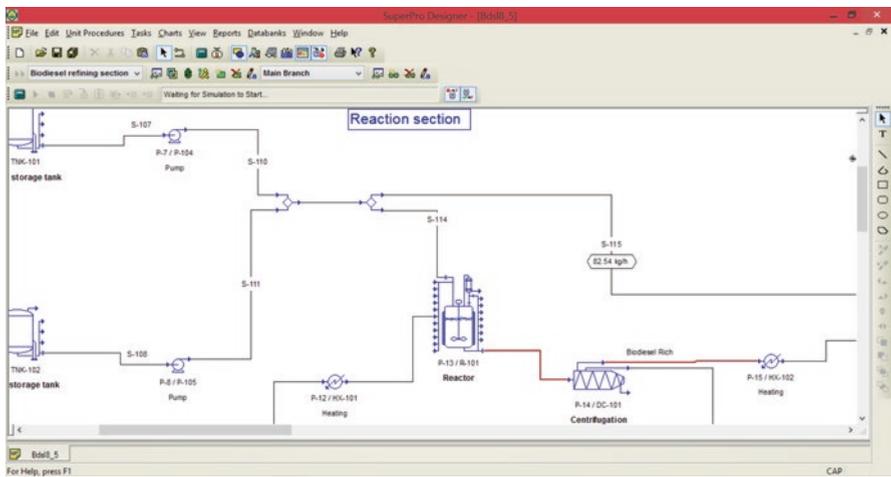**Fig. 7.1** Biodiesel formation reaction

Fig. 7.2 Process flowsheet in SuperPro Designer® for a biodiesel production plant from degummed soybean oil

7.1   Problem Statement

One hundred pounds of fat or oil (such as soybean oil) are reacted with 10 pounds of a short-chain alcohol in the presence of a catalyst to produce 10 pounds of glycerol and 100 pounds of biodiesel. It is a reversible reaction so the short-chain alcohol, signified by ROH (usually methanol, but sometimes ethanol), is charged in excess to ensure quick conversion. The catalyst is usually sodium or potassium hydroxide that has already been mixed with methanol. R', R'', and R''' indicate the fatty acid chains associated with the oil or fat which are largely palmitic, stearic, oleic, and linoleic acids for naturally occurring oils and fats. Part of the process described before is shown in Fig. 7.2.

7.2   Model Formulation

For simplification purposes, the process has been split into three sections: the reaction (blue icons), the biodiesel refining (black icons), and the glycerol purification (green icons) section (Fig. 7.2). A section in SuperPro Designer® is simply a set of unit procedures (processing steps).

Reaction Section
The reaction section consists of:

- The raw material storage tanks for the methanol (TNK-101), the catalyst (TNK-102), and the soybean oil (TNK-103)
- The two reactors (R-101 and R-102)
- A decanter centrifugal separator (DC-101)

The soybean oil is directly fed to the reactor (R-101). Methanol and the catalyst are mixed, and 90% of the mixture is fed to the first reactor. The rest (10%) is fed to the second reactor. According to the reaction mentioned in Fig. 7.1, methanol reacts with soybean oil and yields biodiesel and glycerol. Product is removed at a rate equal to the rate of charging the reactants and catalyst. The average residence time of materials in the reaction is 1 h. Glycerol, a co-product of the acylglycerol transesterification, separates from the oil phase as the reaction proceeds. The reaction extent is approximately 90%. The material is then fed to a centrifugal separator (DC-101) where the biodiesel and the soybean oil that have not reacted are separated from the glycerol-rich co-product phase. The latter is sent to the glycerol recovery unit.

The biodiesel stream, which also contains unreacted methanol, soybean oil, and catalyst, is fed into a second stirred tank reactor (R-102) along with the addition of the methanol-catalyst stream from the splitter (FSP-101). The reaction conditions are the same. The reaction extent in the second reactor is 90% which yields a combined conversion efficiency of 99%.

Again the mixture of methyl esters (biodiesel), glycerol, unreacted substrates, and catalyst exiting the second reactor is fed to another centrifugal separator (DC-102).

Biodiesel Refining Section
This section consists of:

- Two continuous centrifugal separators (DC-102 and DC-104)
- A mixing vessel (V-102)
- A vacuum dryer system (V-104 and GBX-101)
- The biodiesel storage tank (TNK-104)

The crude biodiesel stream is washed with acidified water at a pH of 4.5 in a mixing tank (V-102) to neutralize the catalyst and turn any soap into free fatty acids. The material is then fed to a continuous centrifugal separator (DC-104) to separate

the biodiesel from the aqueous phase, which is fed to the glycerol recovery section. The crude biodiesel product must contain a maximum of 0.050% w/w water. This is achieved by using a vacuum dryer system (V-104 and GBX-101). It lowers the water content from 2.3% to app. 0.04%.

Glycerol Purification Section
This section consists of:

- Two mixing vessels (V-101 and V-103)
- A centrifugal separator (DC-103)
- Two distillation columns (C-101 and C-102)
- Two storage tanks (TNK-105 and TNK-106)

The produced glycerol during the transesterification process requires purification before it can be sold. The equipment is sized to remove methanol, the fatty acids, and most of the product to yield an 80% pure glycerol which is then sold to industrial glycerol refiners at a price of $0.33/kg.

Both glycerol streams (S-119 and S-132) and fatty acid contaminants (S-137) exiting the reactors are pooled and treated with acid (HCl) in V-101 to convert soaps into free fatty acids, which are subsequently removed by centrifugation (DC-103). The fatty acid stream is destined to disposal.

The glycerol stream is then neutralized with caustic soda (in V-103). The methanol contained in the glycerol stream is recovered by distillation (C-101) and recycled back to the first reactor (R-101). Finally, the glycerol stream is concentrated to reach 80% purity by another distillation step (C-102) that removes the water, which is recycled back to the mixing vessel V-102.

7.2.1 Model Simulation Using the SuperPro Designer® Software

This example analyzes the production of 33,635 metric tons (MT) per year of biodiesel using crude degummed soybean oil.

The following SuperPro Designer® flowsheet file has been included with this example:

- Bdsl8_0.spf

This flowsheet shows the base case for the process. The Bdsl8_0.spf file was used to produce the tables and graphs in the rest of this chapter.

Below is a brief description of the basic features of the biodiesel process (file Bdsl8_0.spf). All files for this example can be found in the "C:\Program Files\ Intelligen\SuperPro Designer \ EXAMPLES\BioDiesl" directory.

7.2.2   Definition of the Objective Functions

The gross annual profit (to be maximized) and the environmental impact (to be minimized) of steam power plants are taken as the two objectives to be simultaneously optimized. Next, we present the equations used to calculate these objective functions.

7.2.3   Economic Objective Function

The economic objective function consists in the maximization of the gross annual profit, which represents the difference between the total income and the total annual cost of the biodiesel production plant.

7.2.4   Environmental Objective Function

In this study, the environmental objective function is to minimize the entire CO_2 emissions associated with heating utilities of the biodiesel production plant.

7.3   Stochastic Optimization Algorithm Used

The multi-objective optimization hybrid method, namely, improved multi-objective differential evolution (I-MODE) developed by Sharma and Rangaiah (2013), is used as stochastic algorithm for the optimization of the process in this example.

There were selected four decision variables and introducing a value for the lower and upper boundary. The values of the selected decision variables for the lower and upper bounds, respectively, are 60 and 70 psi for operation pressure in the stream 110, 60 and 70 psi for operation pressure in the stream 111, 55 and 65 °C for operation temperature in the stream 116, and 60 and 70 psi for operation pressure in the stream 116. These values of the decision variables are introduced into the main program user interface of the I-MODE as shown in Fig. 7.3.

For the optimization process, in this case study, the values for the parameters associated with the used I-MODE algorithm are the following: population size (NP) of 100 individuals, generations number (GenMax) of 100, taboo list size (TLS) of 50 individuals, taboo radius (TR) of 0.01, crossover fractions (Cr) of 0.8, and mutation fractions (F) of 0.5. These values of the parameters associated with the used of the algorithm are also introduced into the main program user interface of the I-MODE as shown in Fig. 7.3.
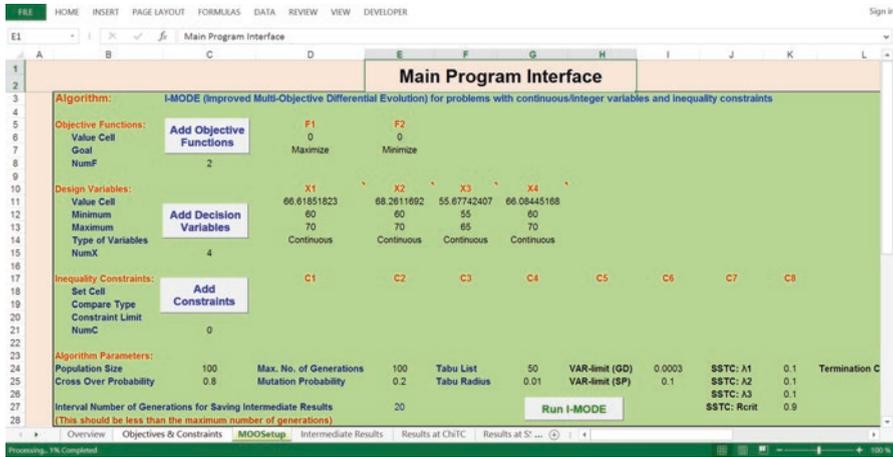
Fig. 7.3 Excel® sheet for the main program user interface of the I-MODE (case 2)
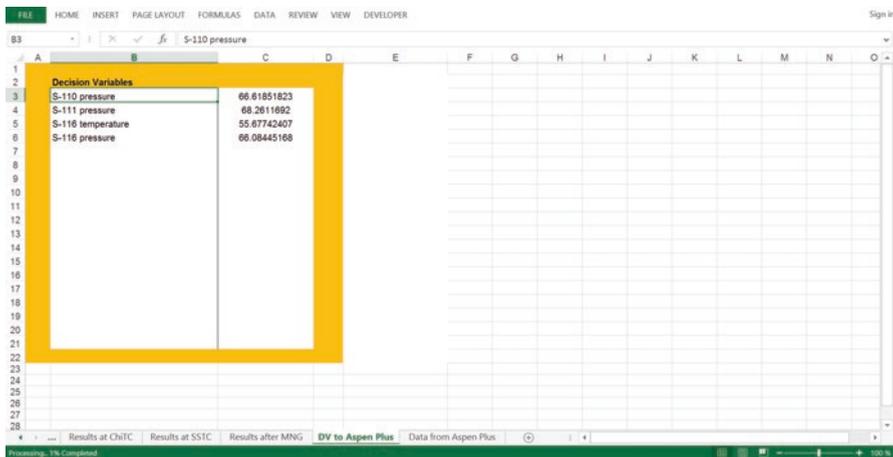

Fig. 7.4 MS Excel® sheet where decision variable values will be sent to the process simulator (case 2)

7.4   Link Between the Process Simulator and Optimization Algorithm

For the adequate link between the process simulator software (Aspen Plus® for this example) and the stochastic optimization algorithm (the I-MODE in this case), it is necessary to follow the methodology mentioned in previous chapters. It is recommendable to add two more MS Excel® sheets, the first one for the decision variable values that will be sent to the simulator (Fig. 7.4) and the second one for the response variable values that will be received from the simulator (Fig. 7.5).
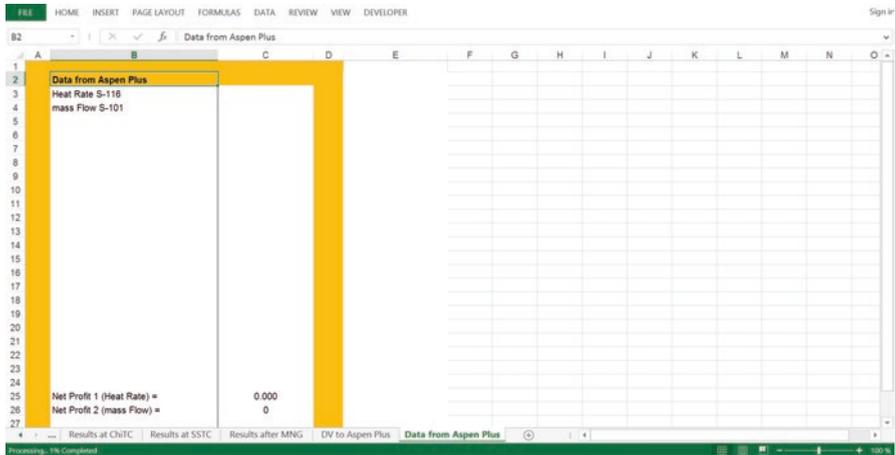
Fig. 7.5 MS Excel® sheet where response variable values will be received from the simulator (case 2)

7.5   Exercises

To download the example of the Generation Power Plant, please click on the following link:

http://extras.springer.com

1. Use the process flowsheet for the biodiesel production from degummed soybean oil implemented in SuperPro Designer® as shown in Fig. 7.2 and implement the following:

   (a) Implement a link between the SuperPro Designer® and the I-MODE algorithm in MS Excel®.
   (b) Analyze the Pareto curves obtained after running the optimization with the same selected decision variables for the lower and upper bounds shown in this chapter.