FUELING THE FUTURE

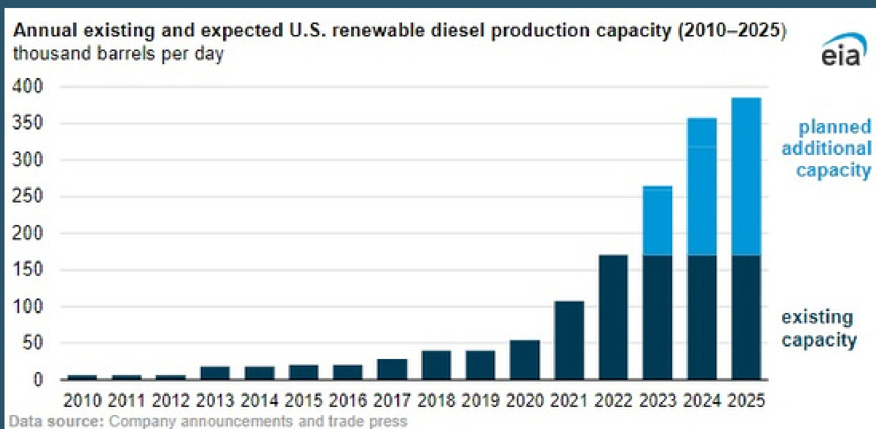
SIMULATION STRATEGIES FOR BIODIESEL PRODUCTION

For more than 30 years, chemical engineers have relied on CHEMCAD, a leading chemical process simulation software, to solve industry challenges. This paper outlines how CHEMCAD helps engineers advance the future of fuels.

CHEMCAD
a datacor product

Fueling the Future

Biodiesel Demand



U.S. Energy Information Administration (EIA)

Net U.S. imports of biodiesel have doubled in the last two years and domestic production of renewable diesel is expected to continue to increase in demand.

Demand is driven by fluctuations in consumer preferences, government regulations, and concerns over energy security. Biodiesel producers looking to take full advantage of the current market must also contend with increased global competition – including from conventional diesel, shorter product lifecycles, rising fuel/feedstock costs, reduced engineering staff, and changes to regulation and public opinion.

The evolving landscape of renewable fuels has illuminated significant value-add opportunity in the optimization of the biodiesel production process(es), including energy usage and reactor conversion, for the many forward-looking biodiesel producers and process development groups.

Process simulations are a starting point for addressing all of these challenges now. This paper will outline the resources required and the advantages/disadvantages for various levels of model fidelity using industry-leading process simulator, CHEMCAD.

Fueling the Future

Process Design Challenges

The challenges associated with process simulation and optimization in biodiesel production depend on what feedstock is used (including how flexible the process can be to varying feedstocks), and the process design, including what equipment will be used.

There are three basic methods of biodiesel production from oils/fats:

1. **Base-catalyzed transesterification**
2. **Acid-catalyzed esterification**
3. **Enzymatic catalysis**

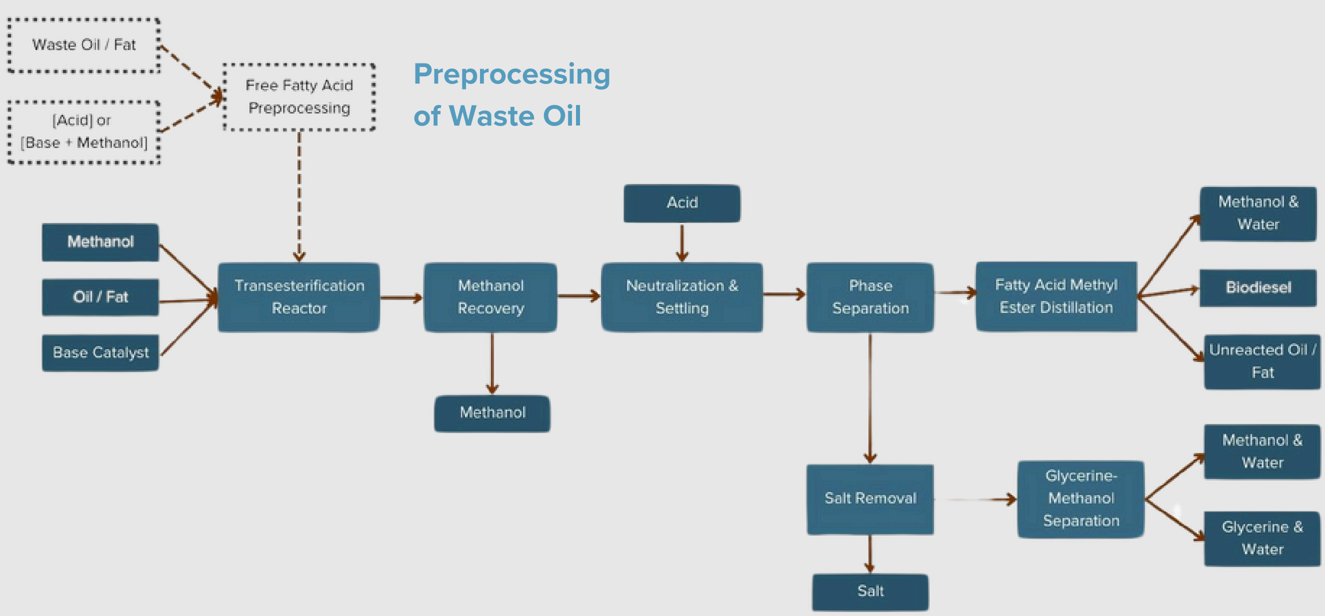
Each reaction has associated optimal operating parameters (T & P) and conversion.

The base-catalyzed process is thought to be one of the better economical routes.

The exact feedstock composition will vary according to the source of the oil/fat and whether it is unused oil or recycled waste oil. When the oil has been used (waste oil), there are usually larger amounts of free fatty acids present than in virgin oils due to the heat from cooking, for example. For biodiesel production, these free fatty acids must be removed with a base or pre-processed with acid esterification to esters before transesterification, to prevent soap formation.

Similarly, depending on the composition of the starting oil/fat, there will be an associated assay of fatty acid esters in the final biodiesel product. The type of alcohol used also determines the type of esters formed. For example, if methanol or ethanol are used, then methyl or ethyl- esters are formed.

Process flow diagram for a base-catalyzed process



Rigorous Method

Biodiesel plant operators can anticipate plant performance with varying compositions and optimize both reaction and separation sections using rigorous simulation in CHEMCAD.

Rigorous simulation, however, requires availability of the physical properties for all oil/fat constituent components, fatty acids, and fatty acid ester products as well as full kinetic parameters for all the reactions (Arrhenius constants).

Additionally, binary interaction parameters will be required for any of the component pairs involved in critical separation processes. These simulation constraints mean rigorous simulation methods require ample available literature data or experimentally measured data, which can be expensive.

Another drawback of the many components and reactions involved in rigorous biodiesel simulation is the computation time required. Even with the parallel processing power of CHEMCAD, the simulation time required can deter some producers seeking optimization opportunities.

Shortcut Method

Due to the drawbacks of rigorous simulation, shortcut methods are often used to model simple heat and material balances for the process.

A common shortcut approach is to use a single, well-documented fatty acid to represent the array of constituent components in a natural oil.

For example, oleic acid is a major component in many vegetable oils, and triolein can be used to represent the triglyceride form of oleic acid.

A low-fidelity model generated with shortcut methods will limit the simulation's ability to accurately model plant performance and perform real-time optimization.

Hybrid Method

If the limitations of low-fidelity shortcut methods and the demands of rigorous modeling are hindering plant performance modeling, a hybrid method may be the preferred approach. In this method, feedstock oil can be represented by a shortened list of fatty acids such as oleic acid, linoleic acid, and linolenic acid. The biodiesel product could then be represented by a shortened list of the fatty acid esters such as methyl oleate, methyl linoleate, and methyl linolenate.

The condensed list of constituent components will still require gathering information such as vapor-liquid-liquid (VLL) binary interaction parameters and the kinetic parameters for the reactions. While a hybrid approach takes some shortcuts by making assumptions about the most critical components and reactions, it offers better fidelity for modeling separation units like distillation and settling/phase separators. In this sort of medium-fidelity model, it will be possible to compare plant performance and optimize both reaction and separation sections of the process.

Fueling the Future

Conclusion

Advanced simulation tools like CHEMCAD can model various feedstock compositions and process conditions to identify the most efficient, cost-effective methods. Producers can use models to anticipate plant performance and optimize the design for changes in feedstock or evolving market conditions. Rigorous, high-fidelity simulation requires an extensive collection of data which may not always be available.

Balancing the detailed accuracy of rigorous simulation with the efficiency of shortcut methods, the hybrid model provides a practical and effective solution. It allows for better fidelity in modeling critical components and reactions, optimizing both reaction and separation units. This medium-fidelity approach ensures that biodiesel producers can achieve reliable and optimized plant performance while managing the complexities of varying feedstock compositions.

References and Further Reading

- U.S. Energy Information Administration (2024, May 28). U.S. biodiesel imports have doubled since 2022 due to low prices in Europe. EIA. Retrieved September 23, 2024, from https://www.eia.gov/todayinenergy/detail.php?id=62123#
- Edwards, John E. Biodiesel Processes in CHEMCAD. Chemstations.com, Oct. 2019
- Zhang, Y., 2002. Design and economic assessment of biodiesel production from waste cooking oil. M.A.Sc. Thesis, Department of Chemical Engineering, University of Ottawa.
- Zhang, Y., Dube, M.A., McLean, D.D., Kates, M., 2003. Biodiesel production from waste cooking oil: 1. Process design and technology assessment. Bioresour. Technol. 89 (1), 1–16.

CHEMCAD
Engineering Advanced

All-in-ONE Software:

Steady-State Models or Dynamic Simulations

- Quickly simulate process scenarios
- Improve safety & regulatory compliance
- Sustainably balance energy & materials
- A single graphical user interface
- Highly customizable & flexible
- Outstanding technical support

35+
Years

80+
Countries

14+
Distribution Partners

400+
Universities

Validate | Calculate | Optimize

CHEMCAD
Engineering Advanced

All-in-ONE Software:
Steady-State Models or Dynamic Simulations

- Quickly simulate process scenarios
- Improve safety & regulatory compliance
- Sustainably balance energy & materials
- A single graphical user interface
- Highly customizable & flexible
- Outstanding technical support

35+
Years

80+
Countries

14+
Distribution Partners

400+
Universities