**Technical Prospectus**

A Research Paper submitted to the Department of Engineering and Society

Presented to the Faculty of the School of Engineering and Applied Science

University of Virginia • Charlottesville, Virginia

In Partial Fulfillment of the Requirements for the Degree

Bachelor of Science, School of Engineering

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On my honor as a University Student, I have neither given nor received unauthorized aid on this assignment as defined by the Honor Guidelines for Thesis-Related Assignments

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In an increasingly mechanized world that demands higher energy usage, the associated environmental impact, including climate change and pollution control, have become dominant global issues. As a result, there is growing concern about automobile emissions and the impact of greenhouse gasses (GHG). These emissions, primarily consisting of $CO_2$, $CH_4$, and $N_2O$, act like a blanket when released into the atmosphere, absorbing the Earth's infrared radiation and preventing heat loss into Space. This accelerates the warming of Earth's surface. To mitigate these effects, the Environmental Protection Agency (EPA) has set an ambitious goal of achieving net-zero GHG emissions across the economy by 2050, aiming to create a clean and affordable mobility system (US EPA, 2023). In 2016, the transportation sector overtook power in GHG emissions (Bleviss, 2021). Since then, GHG emissions from transportation have continued to rise, now encompassing over 28% of global carbon emissions (US EPA, 2015). Therefore, transitioning vehicles to cleaner and more sustainable fuels is vital to reaching the EPA's goal and protecting our planet against climate change.

Biodiesel, made from the reaction of biomass – such as vegetable oils or animal fats – and alcohols, has been seen as a potential alternative to petroleum based diesel fuels (Sheehan et al., 1998). Traditional highway petroleum (low-sulfur) diesel introduces new carbon into the atmosphere that was previously held as underground reserves, such as crude oil. However, biodiesel utilizes carbon sources that have already been in the atmosphere, including carbon absorbed by plants during photosynthesis. In America, most highway diesel sold as gas stations is a 5% biodiesel blend (Hearst Autos Research, 2020). Increasing access to higher percentage blends is key to reducing carbon emissions. While the biodiesel market is on the rise, having produced 21.8 billion gallons in 2024 compared to only 25 million gallons in 2005, its cost remains a hindrance for large-scale adoption (Greer, 2024; Hearst Autos Research, 2020). Figure

1 shows the cost of B100 compared to traditional petroleum diesel prices over the last 11 years (U.S. Department of Energy, 2024). These higher prices are most likely a result of the expensive production methods and raw materials currently in use. (Nagapurkar & Smith, 2023).

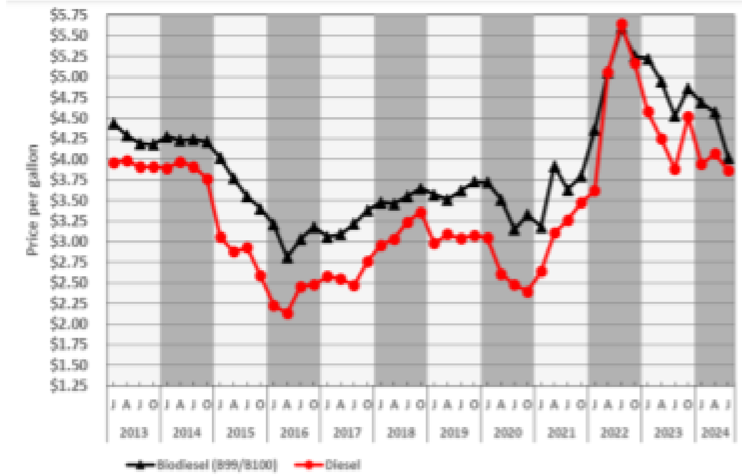


Figure 1: Cost of B100 fuel versus petroleum diesel since 2011. Copied from the U.S. Department of Energy Clean Cities and Communities Alternative Fuel Price Report from July 2024.

Current methods of biodiesel production require the use of alkali, acid, or enzymatic catalysts to transesterify the triglycerides found in the lipids of biomass. This process involves using an alcohol, such as methanol, to help convert these triglycerides into free fatty acid methyl esters (FAME), commonly known as biodiesel (Figure 2) (Zeng et al., 2014). These processes have significant limitations, including slow reaction rates and sensitivity to water and free fatty acids, which increase operation costs (Van Kasteren & Nisworo, 2007; Zeng et al., 2014). Specifically, when free fatty acids found in waste oils react with alkali catalysts, the most common catalyst in use, soaps form. This unsalable waste stream wastes raw materials and reduces methyl ester yield. Also, enzymatic

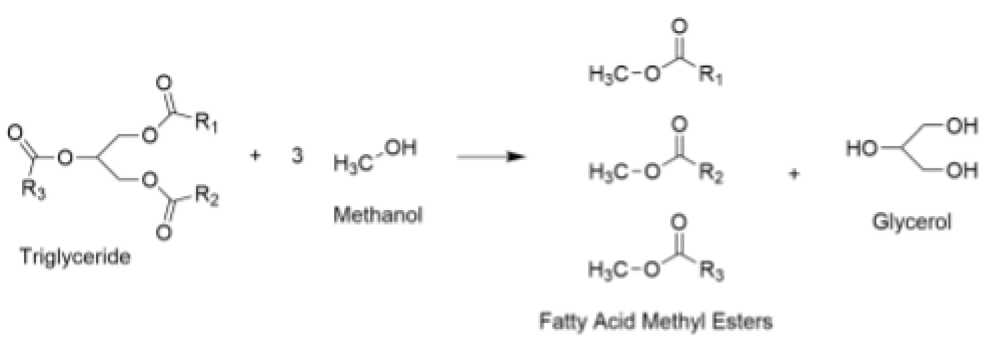


Fig 2. Production of fatty acid methyl esters (biodiesel) and glycerol from the reaction of triglycerides and methanol. Adapted from Van Kasteren and Nisworo (2007)

catalysts, such as lipases, are expensive and deactivate in the presence of methanol (Zeng et al., 2014). Therefore, due to pre-treatment costs to remove water and fatty acids, catalyst maintenance, and catalyst replacement, all catalytic transesterification methods have costly inhibitors to their full adoption in biodiesel production (Nagapurkar & Smith, 2023; Zeng et al., 2014).

However, recent developments in supercritical transesterification pathways have pointed towards potential cost-reductions in biodiesel production. This method capitalizes on the fact that at supercritical conditions, changes in pressure alter the solubility of the reactant and products and cause the fluid, methanol, to behave like both a liquid and a vapor (Zeng et al., 2014). As a result, catalysts are not required to assist in the reaction and the separation of products is simpler (Van Kasteren & Nisworo, 2007). Furthermore, supercritical pathways are insensitive to water and fatty acids which eliminates the need for extensive pretreatment. This allows for lower-grade feedstocks such as waste cooking oil (WCO), the focus of our project, to undergo transesterification, and ultimately lowers feed costs. Overall, when comparing the economic viability of catalyzed vs supercritical transesterification, as represented in Figure 3, the use of a supercritical pathway is the most promising (Brahma et al., 2022; Nagapurkar & Smith, 2023).

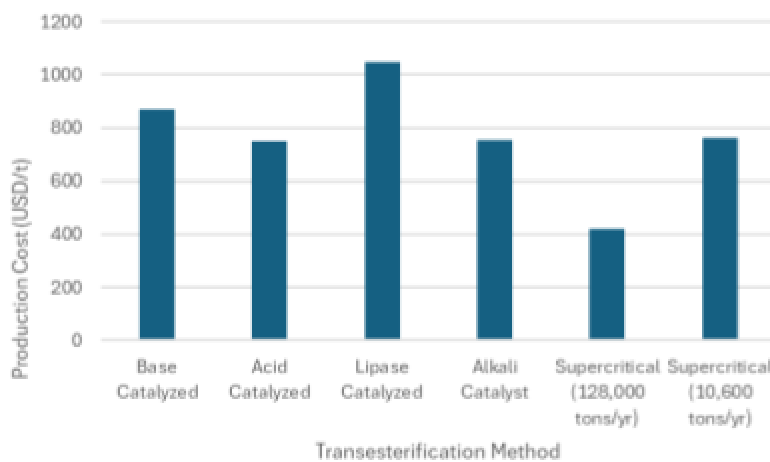


Figure 3: Production cost of biodiesel from WCO. Modeling of supercritical processes shows lowest production cost per ton. Adapted from Brahma et al. (2022) and Nagapurkar & Smith (2023)

The goal of this project is to design and assess the economic feasibility of a biodiesel plant. Biodiesel, conforming to ASTM D6751 biodiesel standards (Appendix A), and pharmaceutical-grade glycerol will be produced via a supercritical methanol transesterification pathway (D02 Committee, 2024). Propane will be used as a co-solvent because it decreases the supercritical temperature and pressure and reduces the required methanol to oil ratio (Van Kasteren & Nisworo, 2007). The basic process operations for this proposal were adapted from Van Kasteren & Nisworo (2007) and Nagapurkar & Smith (2023). WCO and a fresh methanol and propane stream will be combined with a recycle stream containing propane and methanol. The combined stream will be heated and pressurized to approximately 280 °C and 128 bar using thermal energy exchangers (Van Kasteren & Nisworo, 2007). This stream will be fed to an adiabatic plug flow reactor in which the transesterification reaction will take place. Then, the high-pressure products will be expanded in a flash drum to approximately 5 bar, where the unreacted liquid methanol and propane vaporize and are sent to the recycle stream. Remaining

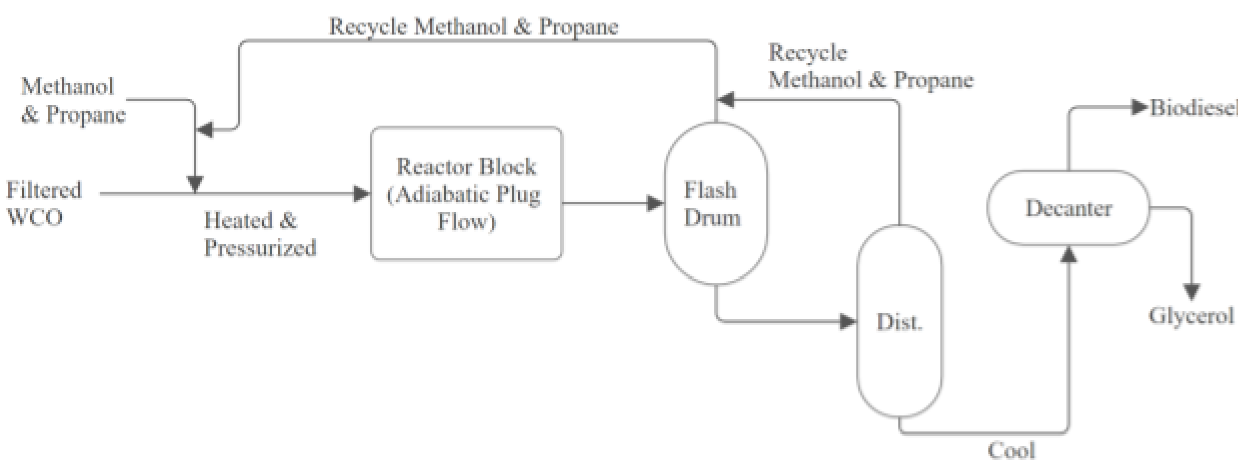


Figure 4: Simplified process diagram for the production of biodiesel from WCO
Adapted from Nagapurkar & Smith (2023) and Van Kasteren & Nisworo (2007)

methanol will be recovered and recycled using a distillation column. The bottoms product of the distillation column will be cooled and sent to a decanter that will separate the biodiesel product from glycerol. Previous studies have shown that it is possible to achieve pharmaceutical-grade glycerol from this process, which will be sold as a profitable by-product (Nagapurkar & Smith, 2023). Figure 4 includes the simplified process design.

The team will use Aspen Plus V14 Simulation software to model the transesterification process for biodiesel production from waste cooking oil (WCO) in supercritical systems. Aspen Plus simulates complex chemical processes using robust thermodynamic models. The Soave-Redlich-Kwong (SRK) equation of state will be used to model the reactor block since it is useful for operations requiring high pressures and temperatures. This model accurately simulates the behavior of methanol in its supercritical state, optimizing the reaction without the need for traditional catalysts. To ensure safety in designing for high-pressure systems, we will consult with Professor Ronald Unnerstall, who brings decades of experience in process safety, particularly in high-pressure environments and the biofuel industry, on necessary safety practices and equipment. His insights will be invaluable in addressing the safety challenges posed by operating under supercritical conditions. For kinetic data, we will leverage past studies on supercritical systems using WCO and other plant oil feedstocks. This data will inform our reaction rates, system design, and overall process efficiency. Specific compositions of WCO and plant siting information will be detailed in the Design Basis Memo in November 2024. The project will take place over two semesters through CHE 4474 and 4476, with the team delegating tasks based on individual strengths and familiarity with specific aspects of the process. Regular cross-checks and collaboration will ensure a cohesive and accurate final design, culminating in a detailed report in April 2025.

## Appendix

*Appendix A: Properties of Biodiesel from ASTM D751 and EN 14214 Standards*

| Properties | ASTM D6751 | EN 14214 |
|---|---|---|
| Flash point, min (°C) | 100–170 | ≥120 |
| Cloud point (°C) | −3–−12 | - * |
| Pour point (°C) | −15–−16 | - * |
| Kinematic viscosity at 40 °C ($mm^2/s$) | 1.9–6.0 | 3.5–5.0 |
| Specific gravity at 15 °C (kg/L) | 0.88 | 0.86–0.90 |
| Density at 15 °C ($kg/m^3$) | 820–900 | 860–900 |
| Cetane number, min | 47 | 51 |
| Iodine number, max | - * | 120 |
| Acid number, max (mg KOH/g) | 0.50 | 0.50 |
| Ash (wt %) | 0.02 | - * |
| Sulphated ash, max % (m/m) | 0.02 | 0.02 |
| Oxidation stability, min (h, 110 °C) | 3 | 6 |
| Water and sediment, max (*v*/*v* %) | 0.05 | 0.03 |
| Water content, max | 0.03 (*v*/*v*) | 500 (mg/kg) |
| Free glycerol, max (mass %) | 0.02 | 0.02 |
| Total glycerol, max (mass %) | 0.24 | 0.25 |
| Sulphur content, max | 0.05% (m/m) | 10 mg/kg |
| Phosphorus content, max | 0.001% (m/m) | 10 mg/kg |

* Not specified.

Copied from Zahan & Kano (2018)

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