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Model for the analysis of the Coprocessing of vegetable oils in a traditional Refinery aimed at the production of Sustainable Aviation Fuel

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The global aviation industry, crucial for global tourism and trade, faces increasing pressure to reduce its environmental impact. Currently responsible for approximately 2.5% of global CO₂ emissions, the sector urgently needs sustainable solutions. This study explores coprocessing vegetable oils in existing petroleum refineries as a cost-effective and scalable method for producing sustainable aviation fuel (SAF). This approach leverages established infrastructure and accelerates the transition to cleaner fuels.

Our model analyses the coprocessing of vegetable oils through catalytic hydroprocessing, validated for up to 5% biomass integration. We use advanced thermodynamic and kinetic modeling to optimize key operational parameters, focusing on the coprocessing of vegetable oils with conventional feedstocks. Careful catalyst selection, particularly Co-Mo and Ni-Mo sulfides, is essential to mitigate challenges like sulfur leaching, coke formation, and diffusion limitations.

This study emphasizes the significant potential for greenhouse gas (GHG) reductions, aligning with the EU’s RED III directive, which mandates a 50-70% GHG reduction compared to conventional jet fuel. Furthermore, integrating digitalization through predictive analytics and monitoring enhances system flexibility and efficiency, enabling refiners to adapt to varying biomass inputs.

The findings demonstrate that coprocessing could be a viable and sustainable pathway for SAF production, empowering in the nest future refiners to meet regulatory requirements and contribute to the aviation sector's net-zero target by 2050. This model provides a valuable tool for industrial implementation and supports the development of energy transition solutions with minimal disruption to existing infrastructure.

* 1. Introduction

Global aviation is essential for economic and social connectivity, yet its carbon footprint is a growing concern. The sector's contribution to global CO₂ emissions, currently around 2.5% (Lau et al., 2024), is projected to rise significantly with the anticipated doubling of air traffic every 15 years. This necessitates the rapid development and deployment of sustainable alternatives. SAF has emerged as a promising solution (Watson et al., 2024). Coprocessing renewable feedstocks like vegetable oils in existing refineries stands out due to its potential for cost-effectiveness and scalability (Bezergianni et al., 2018).

This analysis delves into the technical and operational aspects of coprocessing vegetable oils for SAF production. We examine crucial parameters, including operating conditions, catalyst selection, and the influence of feedstock properties on product quality. Advanced thermodynamic and kinetic modeling will predict product yields, fuel quality, and emissions performance under various operational scenarios.

**1.1 The Imperative for Sustainable Aviation Fuel**

Aviation's contribution to global GHG emissions is substantial, with projections indicating further increases by 2050. The International Air Transport Association (IATA) is committing to a 50% reduction in net CO₂ emissions by 2050 compared to 2005 levels. Achieving this ambitious goal requires a shift to alternative fuels. SAFs, derived from renewable sources, offer a compelling route to decarbonize aviation (Watson et al., 2024).

Traditional jet fuel, derived from petroleum-based kerosene, is a major source of GHG emissions. SAFs can be produced from diverse sustainable feedstocks, such as vegetable oils, used cooking oils, and animal fats (Lau et al., 2024). These "drop-in" fuels are designed for compatibility with existing aircraft engines and fuel infrastructure, minimizing the need for costly modifications (Braun et al., 2024; Kurzawska & Jasiński, 2021).

**1.2 Coprocessing as a Promising Technology**

Coprocessing integrates renewable feedstocks with conventional petroleum feedstocks within existing refinery units. This offers several advantages:

* Infrastructure Utilization: Leverages existing refinery infrastructure, reducing capital expenditures for new biofuel facilities (Bezergianni et al., 2018).
* Feedstock Flexibility: Processes a variety of renewable feedstocks, enhancing flexibility and reducing reliance on single sources (Lau et al., 2024).
* Cost-Effectiveness: Potentially more cost-effective than dedicated biofuel production due to refinery economies of scale (Bezergianni et al., 2018), (Watson et al., 2024).

Coprocessing is particularly well-suited for SAF production, utilizing established refinery processes like hydroprocessing and fluid catalytic cracking (FCC) (Watson et al., 2024), (Bezergianni et al., 2018). These adaptable processes can handle varying feedstock compositions, making coprocessing a flexible and practical strategy.

**2. Coprocessing Technologies and Processes**

Coprocessing renewable feedstocks, such as vegetable oils, in petroleum refineries typically takes place in hydroprocessing (HDT) and fluid catalytic cracking (FCC) units. These units are well-suited for integrating bio-based materials into existing refining operations, allowing for the production of drop-in fuels compatible with conventional fossil-based products. Hydroprocessing is particularly effective for upgrading renewable feedstocks by removing oxygen and improving fuel stability, while FCC can convert heavier bio-derived fractions into lighter, valuable hydrocarbons.

**2.1 Catalytic Hydroprocessing**

Catalytic hydroprocessing plays a key role in refineries, upgrading heavy petroleum fractions by eliminating sulfur, nitrogen, and oxygen while saturating aromatic compounds (Bezergianni et al., 2018). This process is also applied to renewable feedstocks, such as vegetable oils, which primarily consist of triglycerides. During hydroprocessing, these molecules undergo deoxygenation, producing paraffins that serve as crucial components in jet fuel.

Several essential reactions drive hydroprocessing (Mochida & Choi, 2004; Song et al., 2023; Weitkamp, 2012). Hydrodeoxygenation (HDO) removes oxygen from triglycerides, enhancing the stability and energy content of biofuels. Hydrodesulfurization (HDS) eliminates sulfur compounds, reducing harmful emissions and ensuring compliance with environmental regulations. Hydrodenitrogenation (HDN) removes nitrogen species, preventing the formation of nitrogen oxides (NOx) and preserving catalyst efficiency. Lastly, hydrogenation (HYD) saturates unsaturated hydrocarbons, improving fuel quality and storage properties. Together, these reactions enable the production of cleaner and more efficient fuels.

Catalyst selection is critical for hydroprocessing performance. Co-Mo and Ni-Mo sulfide catalysts are commonly used due to their high activity, stability under harsh conditions, and selectivity in promoting desired reactions (Mochida & Choi, 2004). However, coprocessing vegetable oils presents challenges such as sulfur leaching, coke formation, and diffusion limitations due to the larger organic molecules, requiring careful catalyst design and optimization.

**2.2 Fluid Catalytic Cracking (FCC)**

FCC is another key refining process that converts heavy petroleum fractions into lighter, more valuable products such as gasoline and olefins. While traditionally used for petroleum-based feedstocks, FCC can also process renewable oils and fats. It operates by cracking large hydrocarbon molecules at high temperatures in the presence of a catalyst.

In the context of SAF production, FCC can further break down the heavier paraffinic hydrocarbons produced during hydroprocessing, yielding components more suitable for blending into jet fuel. However, processing vegetable oils in FCC poses challenges, particularly due to their high oxygen content, which can lead to increased coke formation and reduced catalyst activity. Additionally, ensuring feedstock compatibility with existing FCC operations is crucial for maintaining process efficiency.

**3. Feedstock Properties and Selection**

**3.1 Petroleum Feedstocks**

Traditional petroleum feedstocks used in refineries include straight-run kerosene and heavy vacuum gasoil (HVGO), both derived from crude oil through different distillation processes.

Straight-run kerosene is a complex mixture of hydrocarbons obtained via atmospheric distillation. It typically contains about 0.07% sulfur and 0.04% nitrogen by weight (Kurniawaty et al., 2018), making it a valuable intermediate for various refining applications.

Heavy vacuum gasoil (HVGO), on the other hand, is a heavier fraction produced through vacuum distillation. It is characterized by its high density and viscosity, as well as significant sulfur and metal content, which can pose challenges in further refining and upgrading processes (Radwan & Nassar’, 1996).

**3.2 Lipid Feedstocks**

Lipid feedstocks, which include vegetable oils, used cooking oils, and animal fats, are promising renewable alternatives for producing SAF (Bezergianni et al., 2018).

* Palm Oil Mill Effluent (POME): A byproduct of palm oil processing. It contains residual oil that can be recovered. POME has high moisture content and a significant biochemical oxygen demand (BOD) (Mahmod et al., 2023; Mohammad et al., 2021). It typically needs pretreatment to concentrate the oil fraction.
* Recovered Used Cooking Oil (RUCO): Used cooking oil that has been filtered and regenerated. RUCO has high content of unsaturated fatty acids, which can be problematic for the stability of the products and requires careful processing to remove metals and contaminants (Mannu et al., 2020; Tumma et al., 2022).
* Animal Fat: Derived from animal waste products. Animal fats contain a mix of saturated and unsaturated fatty acids40. It also has high content of metals and impurities.

**3.3 Key Properties of Feedstocks**

The properties of the feedstocks significantly influence the performance and product quality of the coprocessing units (Mahmod et al., 2023; Mannu et al., 2020). One key aspect is their chemical composition, which refers to the type and structure of hydrocarbons present, including the ratios of saturated, unsaturated, and aromatic compounds. This composition directly affects the reactivity and overall performance of the material.

Viscosity is another important characteristic, as it determines the fluid’s resistance to flow. High viscosity can pose operational challenges, making pumping and mixing more difficult and less efficient.

The water content also plays a crucial role, as excessive water can cause process inefficiencies and contribute to equipment corrosion, ultimately affecting overall system performance.

In addition, the presence of contaminants such as metals, sulfur, nitrogen, and chlorine can negatively impact catalyst performance and reduce the quality of the final product. These impurities may lead to catalyst deactivation and undesirable side reactions.

Finally, the fatty acid profile is particularly relevant in lipid-based feedstocks. The type and proportion of saturated and unsaturated fatty acids influence hydrogen consumption during processing and determine the characteristics of the final product.

**4. Thermodynamic and Kinetic Modeling**

A kinetic model of the hydrodesulfurization (HDT) and hydrodecarboxylation (HDC) sections was developed using Aspen Plus to analyze and assess the feasibility of coprocessing vegetable oils. This model allows for a detailed evaluation of reaction kinetics, process performance, and the impact of integrating renewable feedstocks into conventional refining operations. By simulating key reaction pathways and operating conditions, the study provides valuable insights into the potential challenges and benefits of incorporating vegetable oils in hydroprocessing units.

**4.1 Thermodynamic Modeling**

Accurate modeling of coprocessing requires careful consideration of the thermodynamics of the system. The Soave-Redlich-Kwong (SRK) equation of state is commonly used for simulating processes involving mixtures of hydrocarbons at high pressures and temperatures. The SRK equation provides an acceptable balance between accuracy and computational efficiency.

**4.2 Kinetic Modeling**

Kinetic modeling is essential for understanding and optimizing the reaction rates within the hydroprocessing units.

* **Hydroprocessing Kinetics:** The reactions in hydroprocessing are typically modeled using a power-law rate equation. The reaction rate depends on the concentrations of reactants and temperature, as described by the Arrhenius equation. First-order kinetics are commonly used for modeling HDO, HDN, and HYD reactions. HDS reactions are often better described by a 1.5-order kinetics (Ayodele et al., 2015; Ferdous et al., 2006; Murena, 1997).
* **Hydrocracking Kinetics:** The kinetics of hydrocracking are often described using a lumped model. This approach groups reactants and products into a small number of classes, allowing for simpler reaction networks and kinetic expressions. A lumped model is used for simulating the hydrocracking process, considering five main classes of components: HVGO, diesel, kerosene, naphtha, and gas (Sadighi, 2013).

To accurately simulate these processes, hydrotreating and hydrocracking reactions were implemented in the model using kinetic parameters derived from the literature, covering a total of 28 reactions. A thorough understanding of reaction mechanisms is essential for optimizing coprocessing, as it allows for better control over reaction conditions and product distribution (Mochida & Choi, 2004; Song et al., 2023).

The simulation results provide insight into product yields, with hydrodesulfurization (HDS1) producing desulfurized kerosene, while hydrocracking (HDC) yields gasoline, kerosene, diesel, and an unconverted fraction used as FCC feed.

The kinetic parameters used in the Aspen Plus model (reaction rates, activation energies, pre-exponential factors) were derived from peer-reviewed literature and represent generalized conditions for Co-Mo and Ni-Mo sulfide catalysts. While these parameters provide a good approximation, they may differ from proprietary, site-specific kinetic data used in industrial settings. In particular, the catalyst activity deactivation over time and actual metal contamination levels were not explicitly modelled. Therefore, the predicted SAF yields should be considered optimistic under steady-state ideal conditions.

**5. Simulation Analysis**

**5.1 Simulation Case Study**

Coprocessing was simulated with an additional 5 wt% feed of lipid matrices in the HDS1 and HDC plants, while maintaining the same operational flow. Four different lipid matrices were considered: POME 1, POME 2, RUCO (used cooking oil), and animal fat.

In particular, the simulation will analyze two different coprocessing cases in two existing refinery units:

* **Hydrotreating Unit (HDS1):** The vegetable oil is blended with straight-run kerosene and then hydrotreated. The impact on sulfur and nitrogen removal is considered, as well as the quality of the product. A 5% coprocessing rate is considered.
* **Hydrocracking Unit (HDC):** The vegetable oil is blended with heavy vacuum gasoil, and is first hydrotreated in the HDT section and then cracked in the HDC section of the plant. The simulation considers a 5% coprocessing rate.

To model these processes, Aspen Plus software was used to simulate the reaction sections of the HDS1 and HDC plants. The simulation was developed based on operating data provided by the refinery, including flow rates, pressure, and temperature, ensuring a realistic representation of the industrial conditions. This approach allows for a detailed assessment of the feasibility and impact of integrating vegetable oils into conventional refining operation.

The straight-run kerosene and heavy vacuum gas oil (HVGO) feeds were represented using mixtures of real compounds, selected based on their molecular class and characteristic distillation curves. The distillation curve data were obtained from the refinery's operating manual.

The lumped kinetic model adopted for hydrocracking divides the complex feedstock into five representative pseudo-components (HVGO, diesel, kerosene, naphtha, gas). This simplification facilitates simulation but may not capture the full complexity of feedstock variability and molecular interactions observed in actual refinery operations. For instance, isomerization and ring-opening reactions, important for SAF quality (e.g., freezing point), are not separately modeled, which could lead to deviations in the prediction of product properties.

**5.2 Simulation Results**

The simulation results provide valuable insights into various aspects of the coprocessing operation. The distillation curves of the simulated products were compared with real data, validating the model for both raw materials and final products. The simulation yields converged with real values.

One key outcome is the analysis of product yield, which quantifies the amounts of sustainable aviation fuel (SAF), gasoline, diesel, and other products generated. Additionally, the study assess product quality by examining the chemical and physical properties of the produced fuels, including sulfur content, density, and viscosity.

Furthermore, the impact of coprocessing on reactor temperature profiles is investigated to understand how operating conditions evolve during the process. The conversion rate in hydroprocessing and hydrocracking units is examined to determine the overall efficiency of the reactions. Finally, the study will assess the effectiveness of heteroatom removal, evaluating the extent to which sulfur, nitrogen, and oxygen are eliminated during hydroprocessing.

Comparing the results of the base case (fed only by petroleum oil matrix) and the coprocessing case, the distillation curves obtained from coprocessing are similar to those of the baseline case. However, a slight increase is observed in the final part of the curve, for both processes, due to the presence of n-paraffins from the lipid matrix.

  

c)

a)

b)

*Figure 1: Comparison of Simulated vs. reference distillation curves for different lipid feedstocks.:
a) POME, b) Animal Fat, c) RUCO*

The figure 1 shows the comparison between the simulated product distillation curves and real refinery data for three co-fed lipid sources: (a) POME, (b) Animal Fat, and (c) RUCO. The curves illustrate the degree of alignment between model predictions and industrial outcomes, validating the simulation accuracy. Slight shifts in the final boiling range, particularly in (b) and (c), are due to the presence of linear paraffins from lipid decomposition. These differences help explain variations in fuel stability and freezing point discussed in Section 5.2.

Coprocessing vegetable oils in refinery units leads to several noticeable effects on process conditions and product composition. One key impact is the increase in effluent temperature, particularly in the HDS1 unit, where exothermic reactions from the bio-matrix cause a rise of about 10°C. A similar temperature increase is observed in the hydrotreating section of the HDC unit.

Hydrogen consumption is also significantly higher than in conventional processing, even with a small proportion of lipid feedstock. Additionally, gaseous effluents such as H₂S and NH₃ increase due to the presence of sulfur and nitrogen in the bio-matrix. Another notable effect is water production, which results from hydrodeoxygenation reactions.

The presence of chlorinated compounds in the feedstock leads to the formation of HCl, posing a potential corrosion risk to processing equipment. In some cases, such as coprocessing with POME 1, incomplete denitrification of kerosene is observed, while sulfur content in kerosene is notably reduced during cofeeding. Finally, when using RUCO and animal fat as feedstocks, incomplete oxygen removal occurs, which could affect the stability of the final product.

**5.4 Sensitivity Analysis**

A sensitivity analysis will be performed to assess the impact of varying the coprocessing rate (between 0 and 15%) on the performance of the refinery units, the quality of the products, and the overall process performance. The sensitivity analysis will help identify optimal coprocessing rates that maximize SAF yield while minimizing operational challenges.

To evaluate the operational flexibility and robustness of the coprocessing strategy, a parametric sensitivity analysis was conducted. The input variables included:

* Cofeeding ratio: varied from 0% to 15% by weight
* Reactor effluent temperature: varied within ±20°C of baseline operating conditions

For each scenario, the output parameters monitored included SAF yield (wt%), Total hydrogen consumption (Nm³/h), Effluent temperature (°C), Extent of heteroatom removal: sulfur, nitrogen, and oxygen (wt%) and Water and gas production: as indicators of deoxygenation and degradation.

The simulations were performed in Aspen Plus by adjusting feed composition and reaction temperature for both the HDS1 and HDC units. The distillation curves, product phase distributions, and conversion efficiencies were extracted from each simulation. The model used steady-state convergence criteria and maintained fixed pressure conditions to isolate the effect of the selected variables.

The sensitivity results allowed the identification of non-linear effects, particularly at higher cofeeding ratios (>10%), where conversion efficiency and sulfur removal declined more significantly. Additionally, the increase in effluent temperature confirmed the exothermicity of the reactions, reinforcing the need for effective thermal management strategies under dynamic feed conditions.

The residual fraction of heteroatoms, SAF flow rate and temperature were analyzed.

* **Effects of Chlorinated Compounds:** It was highlighted that the removal of chlorinated compounds is never complete, due to their low concentration in the feedstock and, consequently, the low reaction rate.
* **Trend of Other Heteroatoms:** In the HDS1 unit, the fraction of sulfur-containing compounds decreased as the proportion of bio-feedstock increased. In contrast, the HDC unit showed an increase in sulfurous compounds, with peaks occurring at intermediate cofeeding levels.

Regarding nitrogen and oxygen content, the HDC unit consistently showed no detectable nitrogen- or oxygen-containing compounds. However, in the HDS1 unit, their presence varied depending on the type of feedstock, with fluctuations observed at different processing conditions.

* **Temperature Variation:** An increase in the effluent temperature of the reaction with increasing percentage of cofeeding. As the percentage of cofeeding increases, a corresponding rise in the effluent temperature of the reaction is observed. This temperature variation is primarily due to the exothermic nature of the chemical reactions occurring during the coprocessing of bio-feedstocks with conventional petroleum fractions.
* **SAF Yield:** In the HDS1 unit, the yield of sustainable aviation fuel (SAF) increases as the proportion of cofeeding rises, with the exact yield varying depending on the type of feedstock used. Similarly, in the HDC unit, both SAF and diesel yields increase, but the extent of the increase is influenced by the specific feedstock being processed.

The assumptions mentioned above, especially the use of ideal kinetics and simplified component lumping, could result in an overestimation of SAF yield. For instance, incomplete deoxygenation and partial conversion of unsaturated fatty acids, observed in real units especially with RUCO or animal fats, may reduce the effective SAF fraction. These limitations will be further addressed in future work through calibration with industrial test data.

**6. Challenges and Considerations**

**6.1 Technical Challenges**

Coprocessing vegetable oils presents several technical challenges, primarily due to the variability in feedstock composition, which can affect process stability and product quality. The presence of large organic molecules may lead to catalyst fouling and reduced activity, while oxygen content in the feedstock can promote coke formation, impacting efficiency.

To mitigate catalyst poisoning and corrosion risks from chlorinated, sulfur- and nitrogen-containing compounds in lipid feedstocks, industrial practice often includes pretreatment steps such as filtration, drying, and adsorptive removal of contaminants. At higher cofeeding rates, additional safeguards like guard beds or corrosion-resistant materials may be necessary to preserve catalyst integrity and ensure operational stability.

Catalyst deactivation, primarily due to coke deposition, metal poisoning, and sulfur leaching, represents a major operational concern during the coprocessing of lipid feedstocks. In industrial hydroprocessing units, catalyst regeneration is typically scheduled every 12–24 months, depending on feedstock composition and process severity. However, the introduction of bio-based feeds often accelerates deactivation due to the higher oxygen and metal content. More frequent regeneration cycles (e.g., every 6–12 months) may be required when coprocessing feedstocks such as RUCO or POME unless effective pretreatment is implemented.

Design strategies aimed at mitigating deactivation include the optimization of hydrogen partial pressure, use of guard beds for metal removal, and graded catalyst loading to distribute reaction severity along the reactor bed. These measures are critical for maintaining catalyst longevity and ensuring stable SAF production under continuous coprocessing conditions.

**6.2 Regulatory and Economic Considerations**

The adoption of coprocessing technologies is shaped by regulatory requirements and economic factors. Government mandates for sustainable aviation fuel (SAF) create market incentives, while carbon credit programs enhance economic feasibility by rewarding emission reductions in aviation (Lau et al., 2024), (ENAC Ente Nazionale per l’Aviazione Civile, 2019). However, the cost and availability of renewable feedstocks like vegetable oils play a crucial role in determining economic viability (Lim et al., 2023). Technical constraints currently limit coprocessing to a maximum of 5% bio-jet fuel blending, restricting overall production (Lau et al., 2024). Additionally, SAF must meet ASTM D7566 standards to be compatible with conventional jet fuel, ensuring compliance with industry regulations (Kurzawska & Jasiński, 2021).

**7. Future Directions**

Advancements in catalyst technology will play a key role in improving coprocessing efficiency, with the development of more robust and selective catalysts enhancing reaction performance. Additionally, effective pretreatment methods can help remove contaminants from renewable feedstocks, ensuring greater process stability (Bezergianni et al., 2018).

Innovative approaches to process intensification could reduce both the footprint and capital costs of coprocessing, making it more economically viable. The integration of isomerization processes will also be essential for lowering the freezing point of bio-jet fuels (due to the presence of n-paraffins from the lipid matrix), improving their suitability for aviation. Finally, optimizing coprocessing conditions will maximize bio-jet yield, further increasing the feasibility of incorporating renewable feedstocks into existing refinery operations.

* 1. Conclusions

Coprocessing vegetable oils within traditional refineries represents a feasible and promising pathway for the production of sustainable aviation fuels. This study highlights the technical and operational parameters that must be carefully managed to ensure the successful implementation of this technology.

The adoption of coprocessing, supported by favorable regulations and advanced technologies, can contribute significantly to the decarbonization of the aviation sector, aligning with global climate goals and promoting a sustainable future for air travel. The model developed in this study is a step toward a deeper understanding and optimal use of coprocessing to meet the rising demand for sustainable fuels in aviation. The simulation results should be considered as a starting point in the process design. While the model provides valuable insights and a useful approximation of SAF coprocessing feasibility, some assumptions—such as ideal reactor behavior and generalized kinetics—should be taken into account when interpreting SAF yields for industrial deployment.

This analysis of the coprocessing of vegetable oils in a traditional refinery environment provides valuable insights into the feasibility and challenges of this technology. Through the utilization of advanced thermodynamic and kinetic modeling, this model seeks to contribute to the broader goal of achieving sustainability within the aviation sector, thereby addressing global climate goals and supporting a future of sustainable air travel. The research will also aid in informing policy decisions and strategic choices by industry stakeholders, facilitating the effective integration of biofuels into the existing fuel infrastructure.

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