



PROCESS SIMULATION OF SUSTAINABLE AVIATION FUEL PRODUCTION VIA ETHANOL

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RESUMO

O presente trabalho tem por objetivo realizar uma avaliação da rota de produção do combustível de aviação sustentável (SAF) a partir do etanol, utilizando o simulador de processos DWSIM. A metodologia consistiu na simulação computacional das etapas de desidratação do etanol, oligomerização do etileno, hidrogenação das olefinas e destilação fracionada dos hidrocarbonetos, bem como a análise de sensibilidade destas etapas, com o objetivo de aumentar a eficiência energética do processo. Foram avaliados dois cenários: um cenário base, com reatores de conversão fundamentados em dados da literatura e patentes, e um cenário analítico, que implementou modelos cinéticos para as etapas reacionais e aprimorou os processos de separação. Os resultados demonstram a viabilidade técnica do processo após a análise de sensibilidade, elevando o rendimento mássico do bioquerosene de 10,3% para 21,9% e reduzindo o consumo energético específico de 20,5 kWh/kg para 9,01 kWh/kg. Conclui-se que a implementação dos modelos cinéticos e a análise de sensibilidade do processo, especialmente na etapa de destilação, foram eficazes para aumentar a produtividade e a eficiência energética, gerando um produto final em conformidade com as especificações da norma ASTM D7566. O estudo reforça o potencial da rota ATJ e do uso de simuladores para o desenvolvimento de biocombustíveis, impactando no processo de transição energética global.

Palavras-chave: Combustível Sustentável de Aviação (SAF); DWSIM; Simulação de Processos; ATJ

ABSTRACT

This study aims to evaluate the route to obtain Sustainable Aviation Fuel (SAF) from ethanol, using the DWSIM process simulator. The methodology consisted of the computational simulation of the stages of ethanol dehydration, ethylene oligomerization, olefin hydrogenation, and fractional distillation of hydrocarbons, as well as the sensitivity analysis of these steps, with the aim of increasing the process's energy efficiency. Two scenarios were evaluated: a base scenario, with conversion reactors based on literature and patent data, and an analytic scenario, which implemented kinetic models for the reaction stages and refined the separation processes. The results demonstrate the technical feasibility of the process, as the optimization increased the mass yield of biokerosene from 10.3% to 21.9% and reduced the specific energy consumption from 20.5 kWh/kg to 9.01 kWh/kg. It is concluded that the implementation of kinetic models and process optimization, especially in the distillation stage, were effective in increasing productivity and energy efficiency, yielding a final product in compliance with the specifications of the ASTM D7566 standard. The study reinforces the potential of the ATJ route and the use of simulators for the development of biofuels, impacting the global energy transition process.

Keywords: Sustainable Aviation Fuel (SAF); DWSIM; Simulation Process; ATJ



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INTRODUCTION

The global energy matrix is undergoing transformations through the adoption of new processes to meet growing societal demands. These changes require a balance between technical and economic aspects to ensure sustainable development. At the same time, the global energy landscape faces significant paradigm shifts, driven by the rising production of atmospheric pollutants that affect multiple social spheres and industries.

Within this framework, the aviation sector is now accountable for approximately 2% of global carbon dioxide emissions and about 12% of all emissions from the transportation sector. Consequently, this sector is a prominent subject of research for synthesizing new biofuels that could replace or supplement those currently in use. The goal is to mitigate the effects of greenhouse gas (GHG) emissions, achieving the net-zero, with these efforts being guided by the ICAO.

In response, the development of Sustainable Aviation Fuel (SAF) emerges as a potential solution. SAF is a biofuel produced from plant or animal-based feedstocks, such as waste oils, fats, or alcohols. Its final composition is a mixture of straight-chain and branched hydrocarbons (C₈–C₁₆), with properties comparable to conventional kerosene. SAF is certified under the ASTM D7566 standard, ensuring compliance with aviation fuel specifications.

Among the certified methods, the Alcohol-to-Jet (ATJ) route stands out as an excellent alternative for producing bio-jet fuel at agricultural countries, like Brazil. The ASTM standard for this pathway allows the use of various C₂ to C₅ alcohols, such as ethanol or iso-butanol. This production process consists of four crucial steps, each with a specific objective:

- **Dehydration:** A catalytic, endothermic reaction that converts ethanol into ethylene, releasing water.
- **Oligomerization:** A catalytic, exothermic reaction where ethylene is converted into higher molecular weight olefins (C₄–C₁₂) to produce unsaturated hydrocarbons within the naphtha, gasoline, and jet fuel range.
- **Hydrogenation:** A catalytic, exothermic reaction to saturate the double bonds in the olefins formed during oligomerization.
- **Distillation:** The final purification step, where hydrocarbons are separated based on physicochemical properties like density and boiling point to achieve the desired product specifications.

This study, therefore, aims to investigate and simulate the production process of bio-jet fuel via the Alcohol-to-Jet route using ethanol as the primary feedstock. The main objective is to assess the technical feasibility of this technological route and analyze the parameters influencing the synthesis process, focusing on the mass and energy balances for each stage developed within the DWSIM process simulator.

MODELING AND SIMULATION

This study's methodology involved simulating the production of Sustainable Aviation Fuel (SAF) from hydrated ethanol via the Alcohol-to-Jet (ATJ) route using the DWSIM software. As a first step, the plant's production capacity was established to meet 5% of the national demand for aviation kerosene. For the process simulation, the NRTL (Non-Random-Two-Liquid) thermodynamic model was applied to polar mixtures (water/ethanol), while the Peng-Robinson (PR) model was used for hydrocarbon systems at high pressure and temperature during the oligomerization and distillation stages.

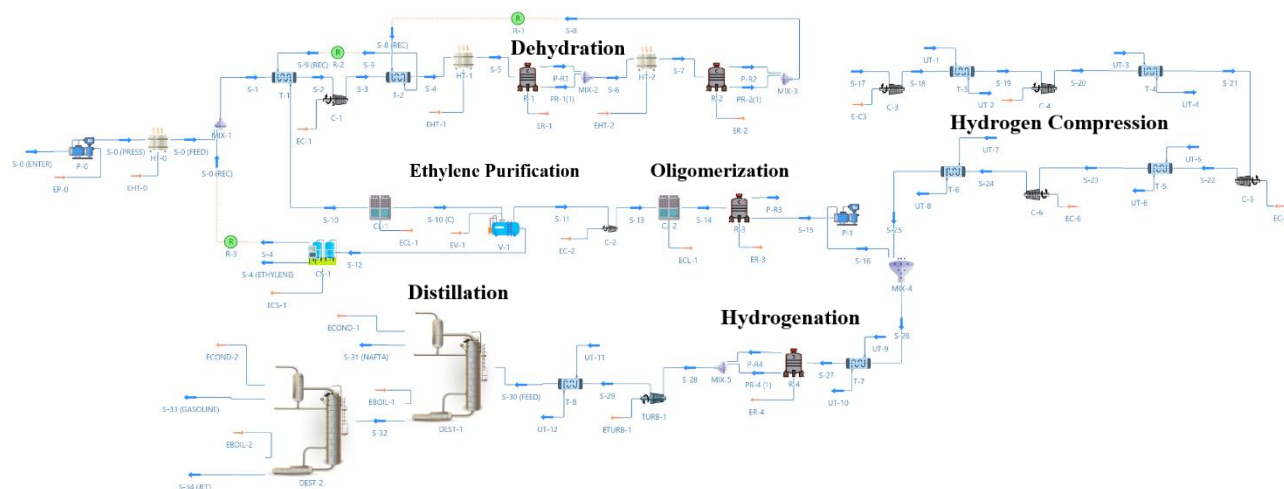


The research was structured into two process scenarios to evaluate the impact of different process conditions on SAF synthesis. The first, the base scenario (Process Scenario 1), was established using operational conditions from academic articles and corporate patents. This allowed for a direct and appropriate adaptation within the process simulator, with the key considerations for each process step described below.

The dehydration, oligomerization, and hydrogenation reactions implemented in the simulator were adapted from the literature, with partial reactions adjusted for each compound. The oligomerization step was simplified to include only the formation of C4–C12 linear olefins, a choice justified by the use of a bifunctional catalyst. After hydrogenation, the distillation stage was modeled with two columns. These columns were simulated using the ‘Shortcut’ method to separate the mixture into naphtha, gasoline, and kerosene fractions, in line with ASTM D7566 specifications.

Given this, Figure 1 illustrates the flowsheet for the synthesis of Sustainable Aviation Fuel in the base scenario (PS1), developed in the DWSIM process simulator, highlighting the main stages of the production process.

Figure 1 – Flowsheet of SAF’s Simulation Process in the base scenario (PS1).



Legend: *Process Streams:* S-1; S-2 ... *Energy Streams:* EP-0; EHT-0 ... *Reactors:* R1; R2; R3; R4 *Heat Exchangers:* T-1; T-2; T-3 ... *Chillers:* CL1; CL2 *Pumps:* P-0; P-1 *Compressors:* C-1; C-2 ... *Pressure Vessel:* V-1 *Mixers:* – MIX-1; MIX-2 ...

The analytical scenario (PS2), focused on process optimization to enhance SAF synthesis efficiency and reduce energy consumption. Key methodological changes included the introduction of kinetic modeling for the reactions, for which rate law models were implemented. The initial analysis employed kinetic models suitable for a ZSM-5 catalyst in a Packed Bed Reactor (PBR), based on single-site and Langmuir-Hinshelwood-Hougen-Watson (LHHW) mechanisms. This model accounted for both the formation of ethylene and the diethyl ether (DEE) byproduct during the dehydration step.

Based on the equations below, the kinetic constants were described using the Arrhenius equation, which is valid within the temperature range of 250 to 400 °C. These constants account for the entire reaction mechanism, including the adsorption of reactants, the surface reaction on the catalyst, and the desorption of the products namely, ethylene from the main reaction and diethyl ether (DEE) from the side reaction, as detailed in Table 1.



Table 1 – Rate Laws for the ethanol dehydration reaction

Chemical Reaction	Expression of the rate	Mechanism
Ethanol to Ethylene	$\frac{k_1(P_A - P_O P_W / K_{eq1})}{(1 + P_A K_{A1})}$	Single-Site
Ethylene to Diethyl-Ether	$\frac{k_2 K_{A2}^2 (P_A^2 - P_W P_E / K_{eq2})}{(1 + P_A K_{A2} + P_E K_{E2})}$	LHHW

Source: Adapted from (WOO, 2021)

Following the ethanol dehydration step, a sensitivity analysis was performed on the operating conditions of the separation vessel. The purpose of this analysis was to purify the resulting ethylene stream and minimize energy consumption by increasing its concentration in the outlet stream as a function of the vessel's inlet temperature.

Additionally, for the oligomerization step, a kinetic model from the literature was implemented. This model is based on power-law kinetics developed for an Al-SBA-15 catalyst operating between 180°C and 230°C at 36 bar. It describes the formation of various olefins, with the specific reactions and their corresponding Arrhenius kinetic parameters detailed in Table 2, including all the secondary reactions.

Table 2 – Kinetic Parameters of oligomerization reaction

Products	Chemical Reaction	Kinetic Law	Arrhenius Equation (J/mol)
But-1-ene (C_4H_8)	$2 C_2H_4 \rightarrow C_4H_8$	$r_1 = k_1 \cdot C_{C2}^2$	$k_1 = 2.277 \cdot 10^{-4} \exp\left(\frac{-109,530}{RT}\right)$
Hex-1-ene (C_6H_{12})	$C_2H_4 + C_4H_8 \rightarrow C_6H_{12}$	$r_2 = k_2 \cdot C_{C2} \cdot C_{C4}$	$k_2 = 1.533 \cdot 10^{-4} \exp\left(\frac{-15,229}{RT}\right)$
Oct-1-ene (C_8H_{16})	$C_2H_4 + C_6H_{12} \rightarrow C_8H_{16}$	$r_3 = k_3 \cdot C_{C2} \cdot C_{C6}$	$k_3 = 3.988 \cdot 10^{-5} \exp\left(\frac{-7,881}{RT}\right)$
	$2 C_4H_8 \rightarrow C_8H_{16}$	$r_4 = k_4 \cdot C_{C4}^2$	$k_4 = 1.914 \cdot 10^{-7} \exp\left(\frac{-44,454}{RT}\right)$
Dec-1-ene ($C_{10}H_{20}$)	$C_2H_4 + C_8H_{16} \rightarrow C_{10}H_{20}$	$r_5 = k_5 \cdot C_{C2} \cdot C_{C8}$	$k_5 = 4.328 \cdot 10^{-5} \exp\left(\frac{-9,438}{RT}\right)$
	$C_4H_8 + C_8H_{16} \rightarrow C_{10}H_{20}$	$r_6 = k_6 \cdot C_{C4} \cdot C_{C8}$	$k_6 = 2.506 \cdot 10^{-7} \exp\left(\frac{-8,426}{RT}\right)$
Dodec-1-ene ($C_{12}H_{24}$)	$C_2H_4 + C_{10}H_{20} \rightarrow C_{12}H_{24}$	$r_7 = k_7 \cdot C_{C2} \cdot C_{C10}$	$k_7 = 4.036 \cdot 10^{-5} \exp\left(\frac{-10,911}{RT}\right)$
	$C_4H_8 + C_8H_{16} \rightarrow C_{12}H_{24}$	$r_8 = k_8 \cdot C_{C4} \cdot C_{C8}$	$k_8 = 1.062 \cdot 10^{-6} \exp\left(\frac{-12,537}{RT}\right)$
	$2 C_6H_{12} \rightarrow C_{12}H_{24}$	$r_9 = k_9 \cdot C_{C6}^2$	$k_9 = 6.055 \cdot 10^{-7} \exp\left(\frac{-7,127}{RT}\right)$

Source: Adapted from (WOO, 2021)

Furthermore, the catalytic hydrogenation of olefins was enhanced by incorporating a recycle stream to purify and reintroduce unreacted hydrogen gas back into the process. Finally, the hydrocarbon separation stage was optimized. The two columns in series from the initial design were replaced by a single column with a side-draw, which reduced the operational energy cost while maintaining final product physicochemical properties comparable to the base scenario.

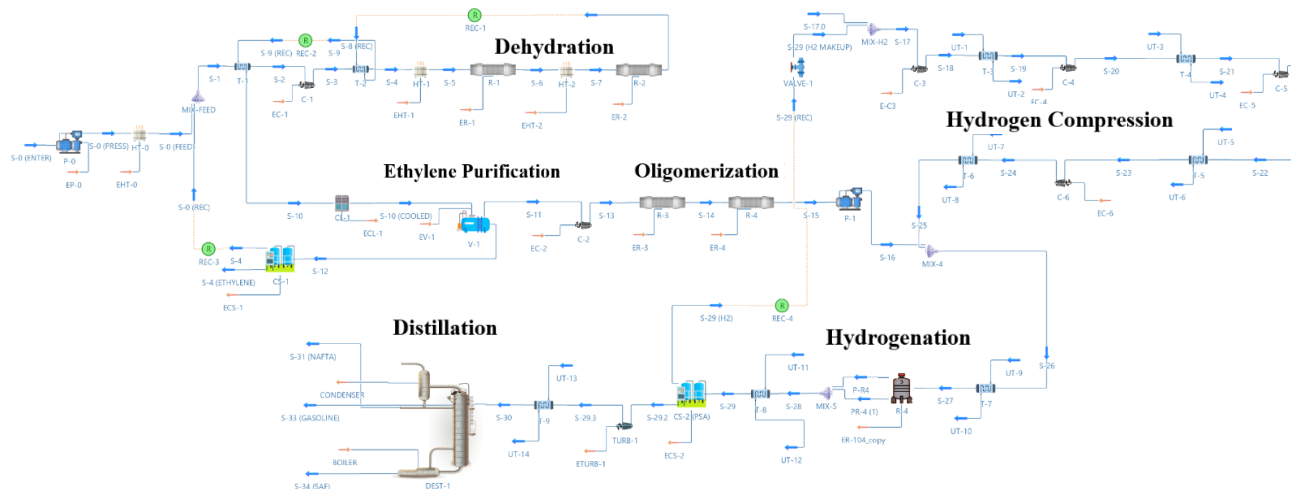


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Analogously to Figure 1, the Figure 2 presents the PS2 scenario, highlighting the key differences in the production process, including the utilization of PBR's reactors, insertion of the hydrogen recycles and optimization of distillation step.

Figure 2 – Flowsheet of SAF's Simulation Process in the analytical scenario (PS2).



RESULTS AND DISCUSSIONS

Based on the methodology presented earlier, partial results were obtained for each stage of the SAF chemical synthesis process, covering both the reaction and the component separation steps. The primary analysis focused on the conversion to the products of interest and the energy consumption of each process stage. This analysis is fundamental for discussing potential improvements for each step.

Initially, focusing on the ethanol dehydration reaction, a comparative analysis highlights the key differences between established literature models and the newly developed kinetic models for the same catalyst. Therefore, in the Table 3, provides a comparison of the conditions process, like the temperature and the partial, global conversion achieved in percentage.

Table 3 – Partial Results – Dehydration Step

Process Scenarios	Reactor (R-1)			Reactor (R-2)			Global Conversion (%)
	Inlet Temperature	Outlet Temperature	Partial Conversion	Inlet Temperature	Outlet Temperature	Partial Conversion	
PS1	400	313	71.5	405	371	97.8	99.4
PS2	400	326	75.1	405	368	71.3	92.8

Source: Elaborated by the Authors based on (AALI, 2022) and (IFP ENERGIES,2020)

The results show that in both scenarios, the overall ethanol conversion exceeded 90% by mass. This demonstrates the technical feasibility of this stage, especially as the kinetic model's performance is comparable to conversion values established in industrial patents. Additionally, the calculated operating temperatures were similar for both the kinetic and the conversion-based reactors, which is consistent with the endothermic nature of ethanol dehydration.



Hence, in the Table 4, the partial results for the ethylene oligomerization stage are presented. The essential point of discussion here is a comparison of the reactor outlet compositions % (m/m) for each component at both scenarios, contrasting the literature-based process conditions with those from the implemented kinetic model.

Table 4 – Partial Results – Oligomerization Step

Olefins synthesized	PS1 (One PBR)	PS2 (Association of PBR in series)	
		Reactor (R-3)	Reactor (R-4)
But-1-ene (C_4H_8)	27.35	28.3	14.6
Hex-1-ene (C_6H_{12})	16.41	55.5	26.0
Oct-1-ene (C_8H_{16})	24.87	11.2	7.4
Dec-1-ene ($C_{10}H_{20}$)	14.92	1.8	14.3
Dodec-1-ene ($C_{12}H_{24}$)	15.92	0.6	35.2

Source: Elaborated by the Authors based on (WOO,2021) and (HEVELING,1988)

The inclusion of a power-law kinetic model, combined with the addition of a PBR reactor in series, increased the formation of higher molecular weight olefins. As a result, SAF productivity improved due to the higher flow rates of C10 and C12 olefins. These compounds are essential for ensuring the desired physicochemical properties of the final fuel.

In the hydrogenation stage, the key results relate to hydrogen recovery, which was achieved using a component separator. This unit, operating similarly to a Pressure Swing Adsorption (PSA) system, was intended to purify the hydrogen from the hydrocarbon stream. So, based on the description above, it's possible to synthesize the partial results of this step, comparison the hydrogen flow rate utilization in both scenarios, including the energy consumption of the systems, presented in the Table 5.

Table 5 – Partial Results – Hydrogenation Step

Process Scenario	Inlet Hydrogen Flow (kg/h)	Recycle Hydrogen Flow (kg/h)	Energy Consumption (KW)
PS1	1,195	0	2,498
PS2	1,351	382	2,889

Source: Elaborated by the Authors

In this context, using a component separator to simulate a Pressure Swing Adsorption (PSA) unit proves to be a practical approach. It allows for a more realistic representation of the catalytic hydrogenation process, enabling the recirculation of approximately 30% of the hydrogen relative to the reactor's inlet stream.

Next, the results for the hydrocarbon distillation step are discussed. This process is crucial for ensuring that the final produced fuels meet the required properties. The PS1 and PS2 scenarios investigated this stage using different distillation column configurations specifically, columns in series versus a single, unified column. These were implemented using the '*Shortcut Column*' and '*Distillation Column*', methods, respectively, presented at Table 6.



Table 6 – Partial Results – Distillation Step

Properties of Process	Distillation Column (PS1) DEST-1	Distillation Column (PS1) DEST-2	Distillation Column (PS2)
Mass flow rate of Nafta (kg/h)	20,677	-	16,855
Mass flow rate of Gasoline (kg/h)	-	24,146	12,995
Mass flow rate of SAF (kg/h)	-	10,003	21,198
Heat Duty - Boiler (KW)	1,557	4,509	3,783
Heat Duty - Condenser (KW)	2,723	4,013	4,507
Density of SAF (kg/m ³)	-	749.5	748.4
Boiling Point of SAF (°C)	-	210	208

Source: Elaborated by the Authors

The analytical scenario (PS2) is notably characterized by an increased mass flow rate of aviation fuel, keeping the same physical properties of SAF comparing with the base scenario. This outcome came at the expense of a decreased flow of Naphtha and Gasoline, which was a direct result of the increased formation of higher molecular weight hydrocarbons. Additionally, adopting the unified distillation column model led to a significant energy consumption reduction of approximately 40%, lowering both the operational and implementation costs compared to the series configuration.

Based on the results discussed above, it is possible to consolidate the findings into a global perspective. In the Table 7, exhibit the results of the energy balances for the partial steps of the production process. With the results, it is possible to discuss about the both similarities achieved and the key advantages of the analytical scenario (PS2) over the base scenario (PS1).

Table 7 – Global Results – Energy Consumption of Base and Analytical Scenarios

Process Scenario	Dehydration (KW)	Oligomerization (KW)	Hydrogenation (KW)	Distillation (KW)	Energy Consumption (KWh/kg SAF)	Mass yield of SAF (%)
PS1	143,448	47,418	2,498	12,802	20.5	10.3
PS2	135,974	41,915	2,889	8,288	9.01	21.9

Source: Elaborated by the Authors

In summary, the sensitivity analyses conducted for each process stage conclude that the analytical scenario (PS2) is more promising for SAF synthesis via the ATJ route. It reduced the production process's energy cost by approximately 44% compared to the base scenario, an improvement driven primarily by the enhanced synthesis of hydrocarbons in the C10-C12 range, which are key to the desired physicochemical properties of SAF.

The implementation of kinetic models in the dehydration and oligomerization stages provided a more realistic process representation. These models accounted for parallel reactions forming undesirable compounds and incorporated rate law data for the various side and series reactions in the oligomerization step, which was further optimized by using a series of PBR reactors. Additionally, unifying the distillation columns and recovering gaseous hydrogen during catalytic hydrogenation represent fundamental operational changes for process optimization, leading to lower energy and chemical reagent costs.



CONCLUSIONS

In this study, the synthesis of SAF via the ATJ route through process simulation in DWSIM was assessed. The implementation of kinetic models and operational optimization were important for the process's enhancement, resulting in a significant increase in productivity and a reduction in energy consumption. This study validates DWSIM's capability to optimize complex processes quickly and efficiently, proving to be an excellent tool for analyzing the SAF production process.

The results obtained include a mass yield of 21.9% and an energy consumption of 9.01 kWh/kg for process scenario 2. These findings demonstrate that the ATJ route from ethanol is both viable and promising for sustainable aviation fuel production. Moreover, the final product meets the requirements of the ASTM D7566 standard. Therefore, the ATJ process using ethanol is favorable to obtain SAF, however future research could expand the analysis to include the evaluation of the economic cost of implementation and operation (CAPEX and OPEX), as well as life cycle and greenhouse gas emissions analyses in comparison with other SAF technological routes (e.g., HEFA and FT-SPK).

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