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Editorial Corner

Process Modelling and Optimization of Palm Oil Biodiesel Production Using Aspen Plus and Response Surface Methodology

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Biodiesel has gained significant attention as a renewable alternative to petroleum diesel due to its biodegradability, reduced emissions, and compatibility with conventional diesel engines. Recent research has focused on enhancing biodiesel production through feedstock optimisation, catalyst development, process intensification, simulation tools, and statistical optimisation techniques. A major trend in the literature is the integration of experimental studies with process modelling tools such as Aspen Plus to improve biodiesel yield and process efficiency [1].

Several studies have focused on optimising transesterification parameters to enhance biodiesel production. Johari *et al.*, [2] reported that microwave-assisted transesterification significantly improved biodiesel production from dairy waste scum oil by reducing activation energy, shortening reaction time, and achieving ASTM-compliant biodiesel. Verma *et al.*, [3] reviewed various feedstocks and identified alcohol-to-oil ratio, catalyst concentration, temperature, and reaction time as key parameters affecting conversion efficiency and fuel properties, emphasising the importance of process conditions.

Aspen Plus has been widely applied to simulate biodiesel production and optimise process performance. Raja *et al.*, [4] modelled esterification and transesterification processes and demonstrated that optimising the methanol ratio improved yield while reducing operating costs. Kick *et al.*, [5] showed that Aspen Plus can reliably predict reaction behaviour, biodiesel purity, and separation efficiency, confirming its value for process design and preliminary optimisation. Doppalapudi *et al.*, [6] integrated Aspen Plus with Response Surface Methodology (RSM) and reported strong agreement between experimental and simulated results, highlighting the methanol ratio as a dominant factor influencing biodiesel yield.

Beyond conventional biodiesel production, simulation has also been applied to broader bioenergy systems. Chaturvedi [7] used Aspen Plus to convert glycerol, a biodiesel by-product, into hydrogen, demonstrating opportunities for waste valorisation and process integration. Jadoon *et al.*, [8] compared different Aspen Plus modelling approaches for biomass gasification and concluded that restricted equilibrium modelling provides the most reliable predictions. Yang [9] demonstrated high biodiesel yield, energy savings, and economic feasibility for waste cooking oil–based biodiesel through integrated Aspen simulation and techno-economic analysis. Dai *et al.*, [10] developed a low-cost soil-based heterogeneous catalyst achieving biodiesel conversions of 98–99%, highlighting

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catalyst innovation as a key pathway for sustainable production.

The literature indicates that biodiesel yield and fuel quality strongly depend on process parameter optimisation, feedstock selection, catalyst performance, and process simulation. Although Aspen Plus and RSM have been widely applied, most studies treat them independently and lack integrated experimental validation. In addition, limited research has focused specifically on biodiesel production from palm oil waste using a combined optimization–simulation approach. These gaps highlight the need for a unified framework integrating experimental production, Aspen Plus simulation, and RSM optimization to improve biodiesel yield, validate process predictions, and enhance scalability.

Central Composite Design (CCD) within RSM was employed to develop a second-order model for two independent variables. The design consisted of four factorial points at coded levels (−1, +1), four axial points at ±α (α = 1.41421) to ensure rotatability, and five replicated centre points at (0, 0) for estimating pure error and model adequacy, resulting in 13 experimental runs. This design enables evaluation of linear, interaction, and quadratic effects while minimising the number of experiments. Rotatability ensures uniform prediction variance at points equidistant from the design centre, improving model reliability. The horizontal coding approach defines a spherical experimental region suitable for detecting curvature and identifying optimal conditions. The resulting dataset supports the development of a quadratic polynomial model with improved predictive accuracy [11].

Aspen Plus is a widely used process simulation software for designing, analysing, and optimising chemical processes. It enables steady-state simulation of reactions, heat and mass transfer, and separation processes using extensive thermodynamic and physical property databases. Process flowsheets are constructed using unit operation blocks such as mixers, pumps, heaters, reactors, distillation columns, and filters, connected through material and energy streams to perform mass and energy balance calculations [12].

In a biodiesel simulation, a mixer is used to combine oil, methanol, and catalyst streams prior to reaction. A pump increases pressure to ensure smooth flow, while a heater adjusts the feed temperature to the desired reaction conditions. RStoic reactors simulate transesterification based on stoichiometric conversion, whereas RCSTR reactors account for reaction kinetics and residence time. Distillation columns separate methanol, glycerol, and biodiesel based on vapour–liquid equilibrium, and filters remove catalyst residues and solids. All chemical components, including methanol, sodium hydroxide, triglycerides, methyl esters, glycerol, and water, are defined using component IDs, chemical formulas, and CAS numbers. For unavailable species, molecular structures are specified to estimate thermodynamic properties. The NRTL thermodynamic model is selected due to its suitability for representing highly non-ideal liquid–liquid systems [13].

Response surface analysis showed that biodiesel yield increased with reaction time and temperature up to an optimum condition. Higher temperatures reduced oil viscosity and lowered the activation energy required for transesterification, thereby enhancing reaction rates. The maximum biodiesel yield of 98% was obtained at 120 minutes and 55 °C. At lower temperatures, the yield decreased due to slower reaction rates and incomplete conversion. However, increasing the temperature beyond 55 °C reduced yield due to intensified saponification [14].

Similarly, biodiesel yield increased with the methanol-to-oil molar ratio up to an optimum of 1:6. At low ratios, insufficient methanol limited conversion due to poor miscibility between oil and methanol. Increasing methanol improved reactant interaction and promoted ester formation. However, excessive methanol (above 1:9) reduced yield by increasing glycerol solubility, promoting emulsification, and shifting the reversible reaction backwards [15].

Catalyst concentration also significantly influenced biodiesel yield. Increasing catalyst loading from 1 to 2 wt.% improved the yield due to enhanced availability of active sites. The maximum yield of 98% was achieved at 2 wt.% catalyst and a 1:6 molar ratio. However, further increases in catalyst concentration and methanol ratio led to reduced yield due to increased viscosity, mass transfer limitations, and soap formation, which hindered phase separation and product recovery [16].

A validation study was conducted to compare experimental and Aspen Plus predicted biodiesel yields. Experiments using palm oil at methanol-to-oil ratios of 1:6 and 1:9 produced yields of 98% and 94%, respectively. Under the same conditions, Aspen

Plus predicted yields of 99% and 94%, demonstrating strong agreement and validating the model. This study demonstrates an integrated approach combining experimental production, Aspen Plus simulation, and RSM optimization for biodiesel production from vegetable oil feedstock. The results confirm that this approach improves process understanding, prediction accuracy, and scalability, supporting the development of efficient and sustainable biodiesel production systems [17].

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