

SUMMARY

Indonesia is one of the world's largest papaya producers, with production reaching 1,281,307 tons in 2025. Papaya seeds, representing 15–20% of fresh fruit weight, are rich in protein, oil, and bioactive compounds. Conventional extraction methods, including maceration and Soxhlet, require long extraction times, high solvent consumption, and may degrade thermolabile compounds. Ultrasound-assisted extraction (UAE) offers faster mass transfer and shorter extraction times, but its performance depends heavily on solvent selection and extraction parameters. Solvent selection for papaya seed oil (PSO) extraction remains largely empirical. Existing group contribution models (GCMs) estimate several thermophysical properties but were not specifically developed for fatty acids and oils. Therefore, this study developed new GCMs for PSO thermophysical properties and integrated systematic solvent selection, extraction evaluation, kinetic and thermodynamic modeling, optimization, PSO and seed characterization, energy and CO₂ assessment, and LCA. The study began with papaya seed separation, cleaning, and drying at 55°C. Solvents were selected according to Hansen solubility parameters (HSPs), boiling point, and safety, health, and environmental (SHE) criteria. Single, binary, and ternary solvent systems were evaluated using Soxhlet extraction for 6 h. Promising solvents were subsequently tested using UAE at 40–50°C, solvent-to-solid ratios of 10:1–30:1, and extraction times of 15–25 min. PSO yield, extraction kinetics and thermodynamics, energy consumption (EC*), CO₂ emissions (ECO₂*), and statistical optimization were evaluated. Extracts were characterized for fatty acids and bioactive compounds, including phenolics, tannins, carotenoids, antioxidants, and vitamin C, while LCA assessed environmental impacts throughout the process. The Alhanif *et al.* models provided better predictions of PSO thermophysical properties than existing GCMs. Systematic solvent selection reduced 50 potential solvents to five based on HSPs, boiling point, SHE criteria, physical properties, cost, and bioactive interactions. Soxhlet extraction showed that solvent mixtures performed better than pure solvents, with the highest yields from ethyl acetate-n-hexane (77.20:22.80 vol%) and n-hexane-acetone-ethanol (64.58:8.13:27.28 vol%), yielding 19.28 ± 0.21 %wt. and 19.15 ± 0.22 %wt., respectively. UAE produced 10.12–14.79 %wt. PSO. ANOVA yielded a significant quadratic model with insignificant lack-of-fit. Temperature and extraction time positively affected yield, whereas solvent-to-solid ratio had a negative effect. Kinetic analysis indicated that Soxhlet extraction was mainly diffusion-controlled, with more than 83% occurring during diffusion. Dimensionless analysis established an empirical correlation between k_m/D_{eff} (*Sh* numbers) and *Sc*, *Re_p*, and *R/ρ* numbers ($R^2 = 0.9581$, $RMSE = 2.16 \times 10^{-7}$) during UAE extraction. Thermodynamically, Soxhlet required higher activation energies (84.25–103.90 kJ/mol), whereas UAE required only 5.54–16.19 kJ/mol due to cavitation-induced cell disruption. UAE also consumed substantially less energy and generated lower CO₂ emissions. Optimization identified 17.02:1 mL/g solvent-to-solid ratio, 50°C, and 16.33 min, producing 14.34% PSO, EC* of 0.0460 kWh/g PSO, ECO₂* of 0.0368 kg CO₂/g PSO, and desirability of 0.9570. Morphological analysis showed that UAE damaged and hollowed the seed structure through ultrasonic cavitation, facilitating PSO release. FTIR confirmed the presence of fatty acids, triglycerides, proteins, phenolics, and structural components. PSO contained mainly oleic acid (71.06%), followed by palmitic (22.46%) and stearic acids (5.33%). The extract contained 0.16 mg GAE/g phenolics and 0.29 mg TAE/g tannins, with low DPPH activity but potential bioactive effects from terpenoids, esters, and sterols. Finally, LCA demonstrated lower environmental impacts for UAE than Soxhlet. Soxhlet solvent extraction produced approximately 24 times greater impacts across most categories. Oven drying was the largest contributor (56% for Soxhlet and 70% for UAE), followed by solvent separation. Overall, the study provides an integrated framework for sustainable PSO extraction. Future work should validate the Alhanif *et al.* model for other oils and fats, replace n-hexane with safer solvents, optimize UAE parameters, validate pilot-scale correlations, conduct techno-economic analysis, investigate PSO bioactives, and explore lower-impact drying methods.

Keywords: extraction; bioactive; papaya seed oil (PSO); solvent selection; sustainability