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OPTIMIZING PROCESS PARAMETERS FOR EFFICIENT SUPERCRITICAL CO_2 EXTRACTION OF SEED OILS: A REVIEW

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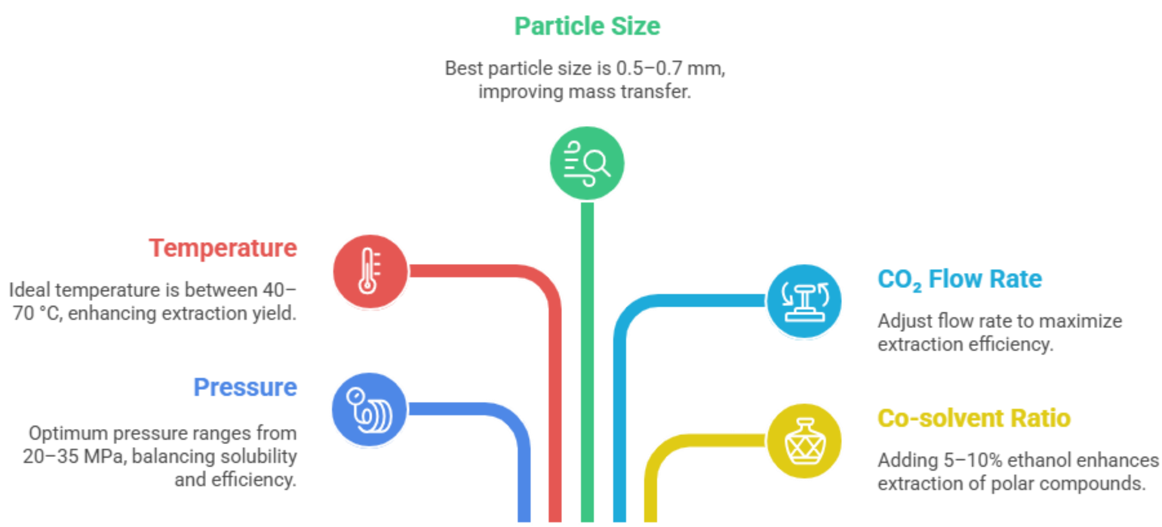
GRAPHICAL ABSTRACT



HIGHLIGHTS

- Key SC-CO_2 parameters significantly influence seed oil yield and quality.
- RSM and ANN effectively optimize multivariable extraction conditions.
- Kinetic and thermodynamic models explain solubility and mass transfer.
- Co-solvents enhance polarity and improve extraction selectivity.
- SC-CO_2 offers green, efficient extraction with strong industrial potential

ABSTRACT

Supercritical carbon dioxide (SC-CO_2) extraction has emerged as one of the most promising green technologies for recovering high-value seed oils enriched with bioactive lipids, antioxidants, tocopherols, and essential fatty acids. As a tunable solvent whose density and solvating power can be precisely controlled through pressure and temperature, SC-CO_2 provides a clean, efficient, and selective alternative to conventional solvent-based extraction methods. This review comprehensively examines the influence of key process parameters—pressure, temperature, particle size, CO_2 flow rate, extraction time, and co-solvent ratio—on oil yield, composition, and functional quality. Across numerous studies, optimal operating conditions typically fall within 20–35 MPa and 40–70 °C, where the balance between solvent density and volatility promotes maximal solubility of triacylglycerols and unsaponifiable compounds. Particle sizes between 0.5 and 0.7 mm consistently enhance extraction efficiency by reducing internal diffusion resistance while maintaining bed permeability and minimizing channeling. The review also highlights the strategic use of 5–10% ethanol as a co-solvent to increase solvent polarity and facilitate the recovery of moderately polar constituents such as phenolics, sterols, and tocopherols. These enhancements are strongly supported by statistical optimization methods, particularly Response Surface Methodology (RSM), which effectively captures interaction effects among variables. Moreover, Artificial Neural Networks (ANN) and Genetic Algorithms (GA) provide powerful nonlinear predictive capabilities, enabling more robust optimization for maximizing yield and tailoring compositional outcomes. To complement experimental findings, empirical and semi-empirical solubility models—including the Chrastil equation, Sovová's mass-transfer model, and the Peng–Robinson equation of state—are widely applied to describe phase behavior, predict solute solubility, and simulate extraction kinetics under varying conditions. The synthesis of current literature confirms that SC-CO_2 extraction offers significant advantages in terms of product purity, environmental safety, and operational selectivity. By eliminating organic solvent residues and supporting energy-efficient processing, SC-CO_2 aligns closely with the principles of green chemistry and the broader movement toward sustainable biorefinery technologies. This review underscores the important role of parameter optimization, modeling tools, and process integration in advancing SC-CO_2 extraction as a scalable and environmentally responsible method for high-quality seed oil production.

Keywords: Supercritical CO_2 extraction; Seed oils; Process optimization; Response surface methodology; Modeling; Green technology; Bioactive lipids

1. Introduction

In recent decades, the demand for natural seed oils rich in bioactive lipids, antioxidants, and essential fatty acids has significantly increased due to their diverse applications in the food, cosmetic, and pharmaceutical industries [1-3]. Conventional extraction techniques often employ organic solvents (e.g., hexane) that pose challenges related to toxicity, solvent residue, environmental impact, and energy inefficiency [4, 5]. Consequently, the need for a cleaner, safer, and more sustainable extraction approach has driven growing interest in supercritical carbon dioxide (SC-CO_2) extraction, which offers a non-toxic, non-flammable, and environmentally benign alternative capable of producing high-purity oils without solvent traces [6, 7].

SC-CO_2 extraction utilizes carbon dioxide above its critical point (31.1 °C and 7.38 MPa), where it exhibits gas-like diffusivity and liquid-like density, allowing efficient solubilization of lipophilic compounds while maintaining moderate operating temperatures [8-11]. These tunable properties make SC-CO_2 particularly suitable for extracting thermolabile compounds, including polyunsaturated fatty acids, tocopherols, sterols, and phenolic antioxidants, from various seed matrices. The technique's versatility enables selective fractionation by adjusting pressure, temperature, and co-solvent composition, providing precise control over both yield and extract quality [12-14]. However, achieving optimal extraction performance requires careful understanding of thermodynamic interactions, mass transfer mechanisms, and solvent–solute equilibria, which are highly dependent on process parameters and seed morphology.

Over the past decade, numerous studies have investigated the effects of operating conditions—including pressure, temperature, CO_2 flow rate, particle size, and co-solvent ratio—on extraction efficiency and oil composition across diverse seeds such as *hemp*, *moringa*, *citrullus*, *pongamia*, and chamomile [15-17]. Optimization methodologies like Response Surface Methodology (RSM), Box–Behnken design (BBD), and Artificial Neural Networks (ANN) have been extensively applied to determine the best parameter combinations for maximizing yield and bioactive recovery. Furthermore, advances in empirical modeling (Chrastil, Sovová) and thermodynamic simulation (Peng–Robinson, SRK) have enhanced predictive understanding of solubility and diffusion behavior under supercritical conditions, enabling more systematic process optimization and scale-up.

This review comprehensively discusses the optimization of process parameters governing SC-CO_2 extraction of seed oils, emphasizing the relationships between thermophysical properties, phase behavior, and extraction kinetics. It also highlights recent developments in modeling, simulation, and hybrid optimization techniques, along with future research trends toward sustainable, energy-efficient, and digitally integrated extraction systems. By consolidating current experimental findings and theoretical advancements, this paper provides an updated framework for researchers and industry practitioners seeking to design high-performance SC-CO_2 extraction processes for functional seed oils.

2. Principles of Supercritical Fluid Extraction (SFE)

Supercritical Fluid Extraction (SFE) is a separation technique that exploits the unique physicochemical properties of fluids above their critical temperature and pressure, where they exhibit characteristics intermediate between those of gases and liquids

[18, 19]. In this state, a supercritical fluid combines the high diffusivity and low viscosity of a gas with the solvent strength of a liquid, allowing efficient mass transfer and selective solvation of target compounds [20]. The process forms the basis for extracting thermolabile and high-value bioactive compounds such as lipids, essential oils, and nutraceuticals from natural matrices.

Carbon dioxide (CO_2) is the most widely employed supercritical solvent due to its moderate critical conditions (31.1 °C and 7.38 MPa), chemical inertness, non-toxicity, and ease of recovery. Above these critical parameters, CO_2 becomes a dense fluid capable of penetrating plant matrices and dissolving nonpolar or slightly polar components such as triglycerides and fatty acids found in seed oils [18]. The solvent power of supercritical CO_2 is directly correlated with its density, which can be tuned by adjusting pressure and temperature [21, 22]. An increase in pressure enhances the density and solubility of lipophilic compounds, whereas temperature variations influence both solute vapor pressure and solvent density, producing complex interactions often termed "crossover behavior." These thermodynamic characteristics make CO_2 a versatile solvent for process optimization [20].

The general SFE process involves three sequential stages: (i) contact of the supercritical solvent with the solid matrix, (ii) solubilization and mass transfer of target compounds into the supercritical phase, and (iii) depressurization and separation of the extract [23]. During extraction, the supercritical CO_2 percolates through the seed bed, dissolving the oil components, which are subsequently separated in the downstream expansion chamber where CO_2 reverts to the gaseous phase, leaving behind solvent-free oil. The process can be operated in static, dynamic, or semi-continuous modes, with dynamic operation being most suitable for industrial applications due to continuous solvent flow and efficient recovery.

The efficiency of SFE depends strongly on parameters such as pressure, temperature, flow rate, particle size, and extraction time, each influencing solvent density, diffusivity, and solute solubility. Optimization of these variables is therefore crucial to achieving maximum extraction yield with minimal energy input. Additionally, the inclusion of co-solvents (e.g., ethanol) enhances the polarity of supercritical CO_2, improving the extraction of moderately polar compounds and broadening the selectivity spectrum.

3. Critical Process Parameters Affecting SC-CO_2 Extraction

3.1. Pressure: Solvent Density, Solubility, and Mass Transfer Effects

Pressure is one of the most critical parameters influencing the efficiency of supercritical carbon dioxide (SC-CO_2) extraction, as it directly affects the solvent's density, solubility, and mass transfer characteristics. In the supercritical region, an increase in pressure substantially enhances the density of CO_2, transforming it into a dense fluid with improved solvent power (Table 1). This high-density CO_2 facilitates stronger molecular interactions with lipid compounds, particularly nonpolar species such as triglycerides, fatty acids, sterols, and tocopherols, thereby promoting higher extraction yields. Numerous studies have demonstrated this positive correlation between pressure and extraction performance. For instance, Minaei, et al. [8] reported that raising the pressure from 100 to 200 bar during coriander seed extraction significantly increased oil yield and linalool purity, while Marčac Duraković, et al. [24] found that fennel seed oil yield tripled as pressure rose to 320 bar. Similarly, Pothinam, et al. [25] observed an optimum of 218 bar for perilla seed oil extraction, yielding 37%, whereas Dhara, et al. [26] achieved nearly 50% PUFA enrichment at 350 bar during garden cress seed oil extraction. These findings collectively confirm that pressure-induced density enhancement is the dominant factor controlling solute solubility and extraction efficiency.

Despite the general trend of yield improvement with increasing pressure, this relationship becomes nonlinear beyond a critical threshold. Once the solvent density reaches near-maximum values, further pressure increments contribute little to solubility gains but considerably elevate energy consumption and operational cost. Studies by Shrirame, et al. [27] and Buranachokpaisan, et al. [28] indicated that pressures above 30–35 MPa resulted in diminishing returns, as the extraction process transitioned from being solubility-controlled to diffusion-limited. Excessively high pressures can also reduce selectivity by co-extracting unwanted waxes or pigments, thereby lowering product purity. Mechanistically, pressure influences SC-CO_2 extraction through three interrelated effects: it enhances solvent density, decreases boundary-layer resistance to diffusion, and shifts the phase equilibrium between CO_2 and oil, modifying the solubility crossover behavior with temperature. Therefore, optimizing pressure is crucial to balance yield, selectivity, and energy efficiency. Most reports converge on an optimal operating window between 20 and 30 MPa, where solvent density and diffusivity are maximized without excessive energy demand. Within this range, SC-CO_2 effectively extracts high-quality seed oils rich in bioactive lipids while maintaining low thermal degradation and high process sustainability, reinforcing the pivotal role of pressure tuning in extraction optimization.

Table 1. Summary of recent studies (2021–2026) showing the effect of pressure on solvent density, solubility, and mass transfer during supercritical CO_2 extraction of seed oils. Increased pressure enhances CO_2 density and solute solubility, improving yield and selectivity; however, beyond an optimal threshold, gains diminish due to diffusion resistance and higher energy consumption.

Authors (Year)	Seed Material	Pressure Range (bar)	Optimum Pressure (bar)	Observed Effect of Pressure on Extraction Yield and Solubility
Minaei, et al. [8]	Coriander seeds	100–200	200	Yield increased with pressure due to higher CO_2 density; 200 bar enhanced terpene solubility and purity while minimizing exergy loss.
Pothinam, et al. [25]	Perilla seeds	200–250	218	Increasing pressure up to 218 bar improved oil yield (37%) and phenolic recovery; further increase gave negligible benefit.
Guta, et al. [29]	Korarima seeds	100–200	155 (15.5 MPa)	Yield rose steadily with pressure up to 15.5 MPa; solubility of terpenes (nerolidol, geraniol) strongly pressure-dependent.
Reinoso, et al. [30]	Maqui & trout oil mix	100–300	300	Extraction yield and omega-3 recovery (EPA, DHA) maximized at 300 bar; pressure intensified solvent power for long-chain lipids.

Authors (Year)	Seed Material	Pressure Range (bar)	Optimum Pressure (bar)	Observed Effect of Pressure on Extraction Yield and Solubility
Marčac Duraković, et al. [24]	Fennel seeds	80–360	320	Overall yield and sterol/tocopherol recovery favored high pressure (320 bar) due to strong density-driven solubility.
Milovanović, et al. [31]	Chamomile seeds	100–450	450	Oil yield increased exponentially with pressure; 450 bar enhanced extraction of unsaturated fatty acids and phenolics.
Pao-La-Or, et al. [32]	Winged bean seeds	150–300	300	Pressure was the dominant variable; yield peaked (36.3%) at 300 bar from enhanced solvation of oleic/linoleic acids.
Dhara, et al. [26]	Garden cress seeds	250–350	350	Higher pressure improved PUFA and tocopherol enrichment; solvent density crucial for selective solubility.
Mazurek, et al. [33]	Blackcurrant & black cumin seeds	200–320	306–282	Yield rose with increasing pressure; near 300 bar, maximum extraction achieved with minimal temperature sensitivity.
Shrirame, et al. [27]	Caraway seeds	150–350	350	Oil yield (3.62%) reached maximum at 350 bar; solubility correlated directly with CO_2 density.
Lukić, et al. [34]	Hemp seed flour	80–200	200	Pressure increase improved extraction efficiency and loading capacity during impregnation; better CO_2 penetration achieved.
Gawron, et al. [35]	Nigella sativa seeds	100–350	35 MPa (350 bar)	Low pressure (10–15 MPa) yielded thymoquinone-rich oil, while higher pressure (35 MPa) improved PUFA recovery.
Buranachokpaisan, et al. [28]	Sesame seed cake	175–225	220	Yield increased with pressure due to higher solvent density; optimal extraction at 220 bar provided rich tocopherol content.

3.2. Temperature: Solubility Crossover & Thermal Degradation Threshold

Temperature plays a pivotal role in supercritical CO_2 extraction by influencing both the solubility and stability of extracted seed oils. Its effect is complex because it governs two competing mechanisms: an increase in temperature enhances the vapor pressure of solutes, thereby increasing solubility, but it simultaneously decreases the density of CO_2, reducing its solvent power. The balance between these two effects produces what is known as the solubility crossover phenomenon, where the dominant effect shifts from density control to vapor-pressure control at a specific pressure. Below the crossover point, higher temperature reduces solubility due to density loss, whereas above it, solubility increases with temperature. Therefore, understanding this interaction is crucial for optimizing oil yield and maintaining product quality (Table 2).

Across the reviewed studies, the optimal extraction temperature for most seed oils lies between 40 and 60 °C, a range that maintains sufficient solvent density while minimizing degradation of thermolabile compounds. For instance, Ferrentino, et al. [36] reported that apple seed oil extraction at 40 °C produced high yields and preserved oxidative stability, while higher temperatures led to reduced density and marginal yield loss. Similarly, Peng, et al. [37] found that Roselle seed oil achieved its maximum yield and γ-tocopherol content at 40 °C, with degradation occurring above 60 °C. Luan, et al. [38] observed a positive influence of temperature on solubility and sterol recovery in *Iris lactea* seeds up to 55 °C, beyond which phenolic compounds began to degrade. These findings highlight the importance of controlling temperature to balance solubility enhancement with the prevention of chemical deterioration.

However, in certain systems, higher temperatures—typically above 70 °C—can temporarily increase mass transfer by reducing oil viscosity and enhancing diffusivity, but this improvement often comes at the cost of thermal oxidation of unsaturated fatty acids. Chouaibi, et al. [39] reported that increasing temperature up to 72 °C improved the yield of *Citrullus colocynthis* oil to 38.12 %, yet further heating risked degradation of antioxidant constituents. Likewise, Priyanka and Khanam [40] achieved a maximum carrot seed oil yield at 70 °C but noted the potential for oxidation of oleic acid under prolonged heating. Suryawanshi and Mohanty [41] demonstrated similar trends for *Argemone mexicana* oil, where higher temperature accelerated diffusion but induced oil darkening—a sign of thermal breakdown. These results confirm that excessive temperature not only lowers solvent density but also triggers degradation of polyunsaturated lipids and tocopherols, compromising oil quality.

Overall, temperature optimization in SC-CO_2 extraction is a delicate balance between improving solubility and preventing thermal degradation. Most studies identify moderate temperatures (40–60 °C) as the optimal operational window, where vapor-pressure enhancement complements sufficient solvent density. Beyond this range, the benefits of faster extraction are offset by oxidative losses and reduced nutritional value. Hence, precise temperature control is essential to ensure that supercritical CO_2 maintains its dual advantage of high solvation power and low thermal impact, leading to efficient recovery of high-quality seed oils.

Table 2. Influence of Temperature on Solubility, Yield, and Thermal Stability during Supercritical CO_2 Extraction of Seed Oils

Authors (Year)	Seed Material	Temperature Range (°C)	Optimum Temperature (°C)	Key Temperature-Related Findings
Chouaibi, et al. [39]	Citrullus colocynthis	40–80	72.4	Increasing temperature enhanced solubility and yield (38.12%) up to 72 °C due to elevated vapor pressure; further heating risks oxidation and reduced antioxidant capacity.

Authors (Year)	Seed Material	Temperature Range (°C)	Optimum Temperature (°C)	Key Temperature-Related Findings
Ferrentino, et al. [36]	Apple seeds	40–60	40	Yield peaked at lower temperature (40 °C); higher temperature reduced density, slightly lowering yield but improved oxidative stability and antioxidant retention.
Priyanka and Khanam [40]	Carrot seeds	50–70	70	Elevated temperature increased oil yield (13.5%) but risked degradation of unsaturated fatty acids at 70 °C; economic feasibility favored moderate heat.
Pavlić, et al. [42]	Raspberry seeds	40–80	50–55	Higher temperature accelerated mass transfer; optimal temperature below 60 °C maintained fatty acid stability and antioxidant quality.
Suryawanshi and Mohanty [41]	Argemone mexicana	60–100	85	Yield increased with temperature up to 85 °C due to enhanced diffusivity; above this, oil darkened indicating onset of thermal oxidation.
Devi and Khanam [43]	Hemp seeds	40–80	76	Moderate-high temperature improved ω-3 and ω-6 fatty acid solubility; excessive heating altered chlorophyll and carotenoid stability.
Bilgiç-Keleş, et al. [44]	Echium vulgare	30–70	62	Yield increased with temperature due to solubility enhancement; beyond 70 °C, degradation of PUFA and tocopherols observed.
Abdullah, et al. [45]	Red pitaya (Hylocereus polyrhizus)	35–65	47	Temperature strongly influenced oil recovery; higher temperature slightly improved yield but reduced unsaturated fatty acid content.
Sodeifian, et al. [46]	Dracocephalum kotschyi	35–65	35	Lower temperature favored oil stability and maintained linolenic acid; elevated temperatures reduced antioxidant retention.
Wejnerowska and Ciaciuch [47]	Quinoa seeds	35–55	40	Oil recovery increased slightly with temperature up to 40 °C; co-solvent addition had stronger impact than temperature alone.
Ndayishimiye and Chun [48]	Citrus by-products	35–55	46	Moderate temperature (46 °C) minimized phototoxic compound (bergapten) formation and maintained antimicrobial activity.

3.3. CO_2 Flow Rate: Residence Time and Mass Transfer Limitations

The CO_2 flow rate is a key operational parameter that strongly influences both the extraction kinetics and efficiency in supercritical carbon dioxide extraction of seed oils. Its effect is primarily associated with mass transfer and residence time of the solvent in contact with the solid matrix (Table 3). An increase in CO_2 flow rate enhances the driving force for solute diffusion and reduces the boundary-layer resistance around seed particles, facilitating rapid solute desorption and transport. However, excessively high flow rates can shorten residence time, leading to incomplete solute–solvent equilibrium and suboptimal extraction yield. Therefore, an optimal flow rate must balance the competing effects of enhanced mass transfer and adequate contact duration to ensure efficient recovery of lipophilic compounds.

Several optimization studies have confirmed that the CO_2 flow rate exerts a nonlinear influence on extraction performance. For instance, Dhara, et al. [26] demonstrated that increasing the CO_2 flow from 20 to 30 g/min improved the yield and enriched polyunsaturated fatty acids (PUFAs) in *Lepidium sativum* (garden cress) oil, as higher solvent throughput enhanced the removal of diffusional resistance; however, flow rates beyond this threshold provided negligible yield gains. Similarly, Shrirame, et al. [27] reported that in *Carum carvi* (caraway) seed extraction, the yield peaked at 14 g/min and declined at higher flow rates due to insufficient residence time for solute dissolution. Buranachokpaisan, et al. [28] observed comparable behavior during *Sesamum indicum* (sesame) oil recovery, where a 5 h extraction at 50 °C and 220 bar achieved 29.8% yield, emphasizing that residence time compensates for moderate flow rates.

In contrast, low flow rates improve equilibrium contact but often reduce the overall mass transfer rate and prolong extraction duration, thereby decreasing throughput and process economy. Ferrentino, et al. [36] found that reducing flow from 8 to 1 L/h for apple seed extraction increased antioxidant retention but slightly lowered yield, while Wejnerowska and Ciaciuch [47] showed that optimal recovery of quinoa oil (89%) was obtained at 40 °C and 25 MPa using moderate flow, as co-solvent addition played a stronger role than extreme flow adjustments. Moreover, Dhara, et al. [26] highlighted that selective extraction can be tuned by manipulating flow: lower flow rates preferentially extract unsaponifiable compounds like phytosterols, while higher flow favors triglyceride recovery. These findings underline the importance of coupling flow optimization with residence time modeling to enhance both yield and selectivity.

Overall, the literature indicates that an optimal CO_2 flow rate typically ranges from 10 to 30 g/min for laboratory-scale systems (corresponding to 0.5–1.5 L/min volumetric flow depending on density and temperature). Within this range, efficient solute transport and near-equilibrium conditions are achieved without compromising energy efficiency or product purity. Excessive flow rates, although improving initial mass transfer, result in increased solvent consumption and diminished extraction economy. Consequently, the interplay between CO_2 flow rate, extraction duration, and system hydrodynamics is central to achieving optimal seed oil recovery in SC-CO_2 extraction processes.

Table 3. Influence of CO_2 Flow Rate on Extraction Yield, Composition, and Kinetic Performance in Supercritical CO_2 Extraction of Seed Oils

Authors (Year)	Seed Material	CO_2 Flow Range	Optimal CO_2 Flow	Notes on Effect
Dhara, et al. [26]	Garden cress (Lepidium sativum)	20–30 g/min	30 g/min (PUFA enrichment) • 20 g/min (phytosterol-rich)	Higher flow boosted PUFA yield; lower flow favored unsaponifiables/selectivity.
Shrirame, et al. [27]	Caraway (Carum carvi)	8–14 g/min	14 g/min	Yield maximized at top of tested range; higher would shorten residence time.
Ferrentino, et al. [36]	Apple seeds	1–8 L/h	1–3 L/h	Moderate flow preserved antioxidants; very high flow slightly reduced yield.
Priyanka and Khanam [40]	Carrot seeds	5–15 g/min	8.53 g/min	RSM optimum balanced yield and solvent use.
Panadare, et al. [49]	Custard apple seeds	1.5–2.5 mL/min	2.5 mL/min (non-volatile) • 1.5 mL/min (volatile)	Fraction-targeted optima: higher flow for non-volatiles, lower for volatiles.
Rai, et al. [50]	Moringa seeds	≈5–15 g/min (0.83×10^{-4}–2.5×10^{-4} kg/s)	— (mid-range recommended)	Mass flow strongly positive up to mid-range; too high cut residence time.
Prakash Maran and Priya [51]	Muskmelon seeds	—	0.64 g/min	RSM optimum for maximum yield.
Mohammed Danlami, et al. [52]	Castor seeds	—	4.15 mL/min	RSM optimum for oil yield.

3.4. Particle Size and Bed Packing Density: Diffusion Resistance and Channeling

Particle size plays a crucial role in determining the efficiency of supercritical CO_2 (SC-CO_2) extraction of seed oils, as it directly influences both mass-transfer dynamics and bed permeability (Table 4). The balance between surface area availability and flow resistance determines the extraction yield and kinetics. In general, decreasing particle size enhances the contact area between the solvent and solid matrix, promoting faster dissolution and diffusion of lipophilic compounds into the supercritical phase. However, excessive size reduction can lead to bed compaction, channeling, and pressure drops, which counteract the benefits of improved diffusivity.

Across the reviewed studies, an optimal particle size typically lies within 0.4–0.8 mm, representing a balance between internal diffusion resistance and external mass-transfer limitations. For instance, Chouaibi, et al. [39] found that *Citrullus colocynthis* seeds with an average size of 0.55 mm achieved the highest yield, as finer particles caused excessive pressure buildup and uneven flow distribution. Similarly, Suryawanshi and Mohanty [41] reported that *Argemone mexicana* seeds showed maximum extraction efficiency at 0.75 mm, where CO_2 permeability was sufficient to prevent local bed compaction.

In the case of smaller seed matrices, fine grinding can be beneficial to shorten diffusion paths. Wang, et al. [53] demonstrated that *Elaeagnus mollis* seeds ground to approximately 80 mesh (≈0.18 mm) exhibited higher oil recovery due to increased surface exposure; however, further reduction below this level impeded solvent flow and reduced efficiency. On the other hand, for *Raspberry seeds*, Pavlić, et al. [42] observed that very small particles (0.3–0.5 mm) accelerated the initial mass-transfer rate but risked channeling, which leads to non-uniform extraction zones.

Other studies confirmed this trade-off. Devi and Khanam [43] optimized *Cannabis sativa* seed oil extraction at 0.43 mm using response surface methodology, indicating that medium-size particles yielded the best ω-6/ω-3 ratio. Sodeifian *et al.* (2018) also found that 0.61 mm particles from *Dracocephalum kotschyi* provided a 71.53% yield, while finer grinding reduced uniformity in CO_2 percolation. Similarly, Abdullah, et al. [45] noted that *Red pitaya* seeds smaller than 0.5 mm caused flow obstruction despite faster kinetics.

Collectively, these findings emphasize that the extraction rate increases with particle size reduction until a critical point is reached, after which hydrodynamic resistance dominates. Therefore, maintaining a moderate particle size range (≈0.4–0.8 mm) ensures optimal mass transfer by minimizing internal diffusion resistance while preserving sufficient CO_2 flow through the extraction bed. This balance is essential for scalable and energy-efficient supercritical extraction processes.

Table 4. Effect of Particle Size and Bed Packing Density on SC-CO_2 Extraction of Seed Oils

Authors (Year)	Seed Material	Particle Size Range	Optimal Particle Size	Key Observations and Notes
Chouaibi et al. (2020)	Citrullus colocynthis	0.30–0.75 mm	0.55 mm	Medium size maximized oil yield and minimized channeling; finer particles led to excessive pressure drop.
Pavlić et al. (2020)	Raspberry seeds	0.3–1.0 mm	0.3–0.5 mm	Smaller size accelerated initial mass-transfer rate; too small produced bed-channeling risk.
Suryawanshi & Mohanty (2019)	Argemone mexicana	0.50–1.00 mm	0.75 mm	Intermediate size favored diffusion without compacting the bed.
Devi & Khanam (2019)	Hemp (Cannabis sativa)	0.30–0.60 mm	0.43 mm	Central composite design identified mid-size as optimal for ω-6 / ω-3 extraction ratio.
Bilgiç-Keleş et al. (2019)	Echium vulgare	Constant (3 kg h^{-1} CO_2 flow)	Not specified	Observed significant effect of temperature–pressure interaction; particle size kept constant.
Abdullah et al. (2018)	Red pitaya	—	0.50 mm	Reduced size improved extraction kinetics; below 0.5 mm risked channeling.

Authors (Year)	Seed Material	Particle Size Range	Optimal Particle Size	Key Observations and Notes
Sodeifian et al. (2018)	Dracocephalum kotschyi	0.15–1.35 mm	0.61 mm	Moderate size gave 71.53 % yield; too small limited flow uniformity.
Suryawanshi & Mohanty (2018)	Pongamia pinnata	0.50–1.00 mm	1.00 mm	Coarser size minimized flow restriction; smaller size increased back-pressure.
Wejnerowska & Ciaciuch (2018)	Quinoa	≤ 0.50 mm	≤ 0.50 mm	Fine grinding (≤ 0.5 mm) greatly enhanced oil recovery (≈ 89 %).

3.5. Extraction Time: Kinetic Profiles and Equilibrium Attainment

Extraction time is a crucial operational parameter that defines the kinetic behavior and equilibrium attainment of supercritical CO_2 extraction. During the process, the extraction rate typically follows a two-stage kinetic profile: an initial constant-rate period controlled by solute solubility in CO_2, followed by a falling-rate or diffusion-controlled stage, where mass transfer becomes limited by solute diffusion through the seed matrix (Table 5). Studies such as those by Minaei, et al. [8] and Pavlić, et al. [42] observed that extraction yield increases rapidly within the first hour and gradually plateaus as equilibrium is approached. The exponential or sigmoidal shape of yield–time curves suggests that most extractable oil is removed during the early stages, making prolonged extraction economically inefficient. In the case of coriander (*Coriandrum sativum*), equilibrium was achieved around 83 minutes with negligible gains beyond 90 minutes, confirming that optimal durations typically lie within 60–150 minutes, depending on the seed structure and solvent accessibility.

In several studies, extraction kinetics were successfully modeled using Sovová's broken and intact cell model, which captures both convection-driven and diffusion-limited transport. For instance, Liu, et al. [54] demonstrated that ultrasound-assisted SC-CO_2 enhanced the initial extraction rate of *Cosmos sulphureus* oil, leading to equilibrium attainment within 75 minutes. Similarly, Sodeifian, et al. [46] reported equilibrium times of 130 and 150 minutes, respectively, for *Dracocephalum kotschyi* and *Elaeagnus mollis* seeds, aligning well with model predictions. These findings indicate that extraction duration must be optimized not only for yield but also for energy efficiency, as prolonged operation offers diminishing returns and increased CO_2 consumption. The rate constants and equilibrium coefficients derived from kinetic models are valuable for scale-up and reactor design, allowing prediction of productivity under different flow and pressure conditions.

The relationship between extraction time and oil yield is also influenced by seed matrix characteristics and solute polarity. In rapidly extractable materials such as *Adansonia digitata* (baobab) and *Perilla frutescens*, equilibrium is reached within 25–60 minutes due to high solubility of free fatty acids and linolenic acid-rich fractions. Conversely, dense or oil-rich matrices like *Sesame cake* require extended extraction periods—up to 300 minutes—to achieve complete oil recovery, although such durations are rarely energy-efficient. Prolonged operation may also lead to degradation or loss of volatile components, as observed by Guta, et al. [29] for *Aframomum corrorima* oil. Overall, the reviewed literature suggests that most SC-CO_2 seed oil extractions reach steady-state equilibrium within 1–2 hours, after which additional extraction time yields minimal improvement. Therefore, defining the optimal extraction duration through kinetic modeling and energy–yield correlation remains essential for achieving cost-effective and sustainable process performance.

Table 5. Effect of Extraction Time on Supercritical CO_2 Extraction Yield, Kinetic Profile, and Equilibrium Behavior of Seed Oils

Authors (Year)	Seed Material	Extraction Time Range	Optimal Time	Key Observations and Notes
Minaei, et al. [8]	*Coriandrum sativum*	30–90 min	83 min	Yield increased rapidly up to ~80 min, then plateaued; steady-state equilibrium reached beyond 90 min; kinetic curve followed exponential saturation behavior; exergy analysis confirmed minimal irreversibility at ~80 min.
Gashi, et al. [55]	*Adansonia digitata*	10–30 min	25 min	Extraction rate limited by solubility rather than mass transfer; equilibrium attained rapidly (< 30 min); short time favored purity and selectivity for free fatty acids.
Pothinam, et al. [25]	*Perilla frutescens*	30–90 min	≈ 60 min	Yield rose sharply within first 60 min and stabilized; extraction kinetics driven by rapid diffusion of linolenic acid–rich fraction; longer durations did not increase yield significantly.
Guta, et al. [29]	*Aframomum corrorima*	60–180 min	147 min	Linear increase up to 120 min followed by equilibrium plateau; prolonged time improved oil yield but risked loss of volatile components; optimal at 147 min for maximum yield (1.6%).
Dhara, et al. [26]	*Lepidium sativum*	30–90 min	60 min	Most oil extracted within first hour; longer times only marginally increased PUFA yield; optimal energy–yield ratio near 60 min.
Panadare, et al. [49]	*Annona squamosa*	30–60 min	60 min (non-volatile) •	Extraction completed within 1 h; distinct kinetic regimes for volatile vs. non-volatile

Authors (Year)	Seed Material	Extraction Time Range	Optimal Time	Key Observations and Notes
			30 min (volatile)	fractions; SEM images confirmed rapid matrix disruption.
Maitusong, et al. [56]	*Foeniculum vulgare (fennel)*	30–90 min	68 min	Oil yield (3.85%) matched model predictions; Sovová kinetic fit $R^2 > 0.98$; equilibrium achieved within 70 min.
Sodeifian, et al. [46]	*Dracocephalum kotschyi*	60–180 min	130 min	Time strongly affected yield up to 130 min; beyond this, system reached equilibrium; modelled using broken-intact cell kinetic model.

3.6. Co-solvent Type and Ratio: Polarity Modulation and Selectivity

The introduction of co-solvents in supercritical CO_2 extraction is a critical strategy for modulating solvent polarity and enhancing the solubility of polar lipophilic compounds. Pure CO_2 is inherently nonpolar (dielectric constant ≈ 1.1), which makes it an excellent solvent for nonpolar triglycerides but relatively ineffective for compounds with moderate polarity such as phenolics, tocopherols, and sterols. By incorporating small amounts of a polar modifier—typically ethanol, methanol, or other protic solvents—the overall polarity and hydrogen-bonding capacity of the supercritical phase increases, facilitating improved extraction of these moderately polar constituents. However, the selection and ratio of co-solvent must be carefully optimized, as excessive polarity can reduce selectivity or co-extract undesirable compounds (Table 6).

A comparison of recent studies reveals distinct co-solvent performance trends (Table 6). Ethanol remains the most widely used modifier due to its green solvent properties, compatibility with CO_2, and ease of post-extraction removal. In *Citrullus colocynthis*, i Chouaibi, et al. [39] identified 8.5% ethanol as optimal for maximizing yield (38.12%) and antioxidant activity, demonstrating the synergy between polarity enhancement and mass transfer. Similarly, *Argemone mexicana* and *Pongamia pinnata* seeds [41, 57] achieved their highest yields at approximately 9% ethanol, confirming that modest co-solvent ratios (< 10%) are sufficient to overcome solubility limitations without compromising the supercritical nature of CO_2. For *Hemp* oil, Devi & Khanam (2019) found that adjusting ethanol flow to 8% selectively influenced the ω-6/ω-3 ratio, suggesting co-solvent use as a compositional steering tool rather than merely for yield enhancement.

Conversely, excessive co-solvent addition can diminish selectivity. In tocopherol-rich *Canola* oil extraction, Sun, et al. [58] observed that ethanol reduced tocopherol concentration, indicating that neat SC-CO_2 provided better selectivity for nonpolar antioxidants. Likewise, Priyanka & Khanam (2020) noted that only a moderate co-solvent addition (≈ 5.9 wt %) improved carrot seed oil yield, whereas higher levels were unnecessary. Some systems benefit from stronger polarity modification: Wejnerowska & Ciaciuch (2018) achieved an exceptional ~89 % recovery of *Quinoa* oil using 20% MeOH/EtOH (1:1) co-solvent with fine grinding (≤ 0.5 mm), showing that combined mechanical and polarity control yields the highest recovery for dense matrices.

Alternative approaches include lipidic co-solvents. Gao *et al.* (2010) demonstrated that using medium-chain triglycerides (MCT, 1.5% w/w CO_2) as a continuous co-solvent in marigold extraction enhanced the recovery of lutein esters—compounds poorly soluble in polar alcohols—while maintaining extract quality. Similarly, Milovanović, et al. [31] reported that re-extraction of *Chamomile* seed residues with ethanol enriched phenolics and unsaturated fatty acids, highlighting a two-stage extraction strategy: neat SC-CO_2 for nonpolar lipids followed by polar-modified CO_2 for residual bioactives.

In summary, the optimal co-solvent concentration generally falls between 5% and 10% ethanol relative to CO_2 flow, where sufficient polarity enhancement occurs without phase instability. Ratios beyond 20% favor total recovery but compromise selectivity and environmental efficiency. Proper co-solvent tuning thus remains central to balancing yield, selectivity, and sustainability in SC-CO_2 seed-oil extraction systems.

Table 6. Effect of Co-solvent Type and Ratio on SC-CO_2 Extraction of Seed Oils

Authors (Year)	Seed Material	Co-solvent Type	Tested Range / Ratio	Optimal Setting	Polarity/Selectivity Impact & Notes
Milovanović, et al. [31]	Chamomile	Ethanol (re-extraction)	Not stated (added in second pass)	Not specified	Ethanol co-solvent re-extraction boosted total yield (to 18.6%) and enriched phenolics/UFAs; useful after neat pass to strip more polar bioactives.
Priyanka and Khanam [40]	Carrot	(Type not specified in abstract)	0–10 wt%	≈5.9 wt%	Moderate co-solvent level maximized yield (13.5 wt%); shows classic gain from slight polarity increase.
Suryawanshi and Mohanty [41]	Argemone mexicana	Ethanol	0–10% of CO_2 flow	9%	Ethanol most influential factor; higher polarity improved overall yield (42.9%) at 85 °C/305 bar.
Devi and Khanam [43]	Hemp	Ethanol	As % of CO_2 flow	8%	Tuning ethanol set ω-6/ω-3 ratio (2.11–3.17); co-solvent used for compositional steering more than gross yield.
Wejnerowska and Ciaciuch [47]	Quinoa	MeOH/EtOH (1:1, w/w)	20% (added to seed)	20%	Co-solvent + fine grind (≤0.5 mm) gave ~89% recovery—biggest jump among co-

Authors (Year)	Seed Material	Co-solvent Type	Tested Range / Ratio	Optimal Setting	Polarity/Selectivity Impact & Notes
					solvent studies; strong polarity lift.
Chouaibi, et al. [39])	*Citrullus colocynthis*	Ethanol	Ethanol concentration varied	8.5%	ANN/RSM optimum included moderate ethanol, balancing yield and antioxidant potency.

4. Experimental Design and Optimization Approaches

Optimization of supercritical CO_2 extraction is a multivariate engineering problem, where yield, purity, and energy consumption depend on several interacting parameters—pressure, temperature, particle size, co-solvent ratio, and extraction time. To handle this complexity, researchers increasingly rely on structured experimental design and modeling frameworks to identify optimal operating conditions and to elucidate the interactions among process variables. This section summarizes the main experimental design tools and computational approaches employed in SC-CO_2 seed oil studies, highlighting their methodological contributions and performance insights.

4.1. Design of Experiments (DOE) Framework in SC-CO_2 Studies

The Design of Experiments (DOE) approach serves as the foundation for process optimization in SC-CO_2 extraction research. DOE systematically evaluates the effect of multiple factors and their interactions using a minimal number of experimental runs. Studies such as Suryawanshi and Mohanty [41] and Devi and Khanam [43] exemplify DOE application in optimizing Argemone mexicana and Hemp seed extractions, respectively. In these studies, pressure, temperature, and co-solvent ratio were treated as independent factors, while extraction yield and compositional quality (ω-6/ω-3 ratio) were dependent responses.

By employing DOE, researchers can quantitatively model nonlinear effects such as retrograde solubility—where yield decreases beyond a critical temperature despite constant pressure—and determine how interactions (e.g., temperature–pressure coupling) shape mass-transfer efficiency. This approach allows efficient exploration of large parameter spaces, enabling predictive modeling of extraction performance under diverse conditions without exhaustive empirical testing.

4.2. Response Surface Methodology (RSM) for Multivariate Optimization

Response Surface Methodology (RSM) remains the most widely used statistical optimization tool in SC-CO_2 studies due to its ability to represent non-linear dependencies and interaction effects between multiple variables. For instance, Chouaibi, et al. [39] applied RSM and compared it with an artificial neural network (ANN) model for *Citrullus colocynthis* seed oil extraction. Their three-level Box–Behnken design identified pressure (275 bar), temperature (72.4 °C), and ethanol concentration (8.5%) as optimal, achieving a 38.12% yield and strong antioxidant activity (IC_{50} = 0.17 mg/mL).

Similarly, Minaei, et al. [8] optimized coriander seed extraction using a Box–Behnken design over temperature (35–45 °C), pressure (100–200 bar), and time (30–90 min), achieving high linalool selectivity (79.1%) at 200 bar, 43 °C, and 83 min. Pothinam, et al. [25] and Guta, et al. [29] also used RSM to determine optimal perilla and korarima seed oil extraction conditions, respectively, demonstrating RSM's robustness in modeling temperature–pressure–time interactions. RSM's key advantage is its empirical polynomial representation, allowing visualization of response surfaces and rapid identification of global optima. The method is particularly effective for single-objective optimization, such as maximizing yield or target compound concentration, under controlled energy input.

4.3. Taguchi and Box–Behnken Designs for Parameter Screening

The Taguchi method and Box–Behnken design (BBD) are specific DOE strategies tailored for different research purposes. The Taguchi method focuses on robust parameter screening with fewer runs and noise-tolerant settings, as demonstrated by Liu, et al. [54] in ultrasound-assisted SC-CO_2 extraction (UASCE) of *Cosmos sulphureus* seed oil. By analyzing signal-to-noise ratios across temperature (55 °C), pressure (25 MPa), and ultrasound energy density, Taguchi optimization produced a maximum yield of 193.1 mg/g within 75 min—highlighting its suitability for hybrid extraction process evaluation.

Conversely, the Box–Behnken design is preferred for model building and interaction analysis. For instance, Reinoso, et al. [30] employed BBD to optimize enzymatic interesterification of maqui and trout belly oils in an SC-CO_2 medium, while Mazurek, et al. [33] and Suryawanshi and Mohanty [41] used BBD to establish quantitative relationships among pressure, temperature, and extraction time. These studies demonstrate that BBD efficiently captures second-order interactions (e.g., pressure × co-solvent, temperature × time) critical for fine-tuning extraction selectivity.

4.4. Artificial Neural Networks (ANN) and Genetic Algorithms (GA) in Process Optimization

Machine learning and bio-inspired optimization techniques have emerged as powerful tools for modeling nonlinear and multivariate phenomena in SC-CO_2 extraction. Suryawanshi and Mohanty [57] first demonstrated the predictive capacity of an ANN model for *Argemone mexicana* oil extraction, achieving a high correlation ($R^2 = 0.9838$) and low mean-square-error (0.0038) in cumulative extraction yield prediction. The ANN's feed-forward backpropagation structure with six hidden neurons successfully captured complex interdependencies among parameters such as temperature, pressure, and ethanol co-solvent ratio.

Similarly, Chouaibi, et al. [39] compared ANN with RSM for modeling *Citrullus colocynthis* seed oil extraction and found ANN offered superior predictive accuracy, reducing estimation error and better fitting the nonlinear yield–temperature–pressure surface. Additionally, Pao-La-Or et al. (2023) introduced a hybrid RSM–Probabilistic Neural Network (PNN) approach for *Psophocarpus tetragonolobus* seed oil extraction, combining statistical design efficiency with data-driven prediction accuracy. Their model reduced computational effort while achieving an optimal yield of 36.27% at 30 MPa, 55 °C, and 90 min, proving the efficacy of hybrid optimization frameworks in predicting extraction performance.

4.5. Hybrid and Multi-objective Optimization (Yield, Quality, Energy)

Modern SC-CO_2 studies are evolving toward multi-objective optimization, where simultaneous maximization of yield and bioactive quality must be balanced against energy and solvent consumption. Minaei, et al. [8] integrated energy–exergy (2E) analysis into their RSM framework, revealing that the liquid-CO_2 pump contributed 42% of total exergy destruction and that stabilizing pump pressure near 150 bar could reduce exergy loss by 14%. Their staged SC-CO_2 system achieved energy efficiency of 32% and exergy efficiency of 27%, with specific energy consumption of 0.62 kWh/kg oil—comparable to industrial best practices.

Such multi-objective frameworks are critical for scalable process design, where trade-offs between productivity and sustainability must be quantitatively defined. In hybrid designs combining ANN or GA with RSM, optimization can be tuned to minimize operational cost or CO_2 consumption while maintaining high extract purity—an approach gaining traction in recent nutraceutical and cosmetic oil applications.

4.6. Validation and Predictive Model Performance Metrics

Model validation ensures that optimized SC-CO_2 conditions yield reproducible and transferable results. Commonly reported metrics include the coefficient of determination (R^2), average absolute relative deviation (AARD%), and root mean square error (RMSE). For instance, Suryawanshi and Mohanty [57] reported AARD = 3.33% and R^2 = 0.9838 for their ANN model, confirming high predictive reliability. Similarly, Chouaibi, et al. [39] obtained strong model alignment between predicted and experimental yields using ANN and RSM, validating the statistical significance ($p < 0.05$) of fitted parameters.

Beyond statistical validation, recent studies (e.g., Minaei, et al. [8]) also apply thermodynamic consistency checks and energy–exergy audits to cross-verify model predictions with physical feasibility, particularly for industrial scaling. The use of experimental confirmation runs at optimized settings (e.g., ± 5% deviation tolerance) is now standard in SC-CO_2 optimization research, ensuring that predictive models remain robust across small perturbations in process variables.

5. Modeling and Simulation of SC-CO_2 Extraction

Modeling and simulation form the scientific backbone of supercritical CO_2 (SC-CO_2) extraction research, enabling prediction, optimization, and scale-up of extraction performance without extensive empirical testing. These models provide mechanistic insight into solubility behavior, mass-transfer kinetics, and thermodynamic interactions under supercritical conditions. In seed oil systems—where lipid classes, fatty acid distributions, and matrix porosity vary considerably—accurate modeling ensures efficient process control and sustainable design.

5.1. Solubility Modeling Using Empirical and Semi-Empirical Correlations (Chrastil, Sovová, del Valle–Aguilera)

Solubility of solutes in supercritical CO_2 is the key determinant of extraction efficiency and selectivity. Empirical and semi-empirical correlations are frequently applied to describe solute–solvent equilibria in SC-CO_2 extraction of seed oils. The Chrastil model relates solute solubility (y) to solvent density (ρ), temperature (T), and vapor pressure, assuming formation of solvato-complexes between solute and CO_2 molecules. For example, Priyanka and Khanam [40] successfully used Chrastil's correlation to describe the yield variation of carrot seed oil across 20–40 MPa and 50–70 °C.

In contrast, the del Valle–Aguilera model incorporates solvent density and sublimation pressure, improving accuracy at high pressure (> 300 bar). Meanwhile, the Sovová mass-transfer model couples solubility data with extraction kinetics, dividing the bed into "broken" and "intact" cells to describe the transition between solubility-controlled and diffusion-controlled regimes. Rai, et al. [59] applied this approach to sunflower seed oil extraction, obtaining an excellent fit ($R^2 > 0.98$) between experimental and simulated yields. Overall, semi-empirical models remain the benchmark tools for predicting solubility in SC-CO_2 systems, though they require careful parameter fitting and experimental calibration for each matrix and operating window.

5.2. Kinetic Models for Seed Oil Extraction (Constant and Variable Diffusion)

Kinetic modeling provides quantitative understanding of mass-transfer mechanisms in SC-CO_2 extraction, which typically follows two distinct stages: a rapid solute-washing phase dominated by external film diffusion, followed by a slower diffusion phase governed by internal mass transfer. The Sovová model remains the most widely accepted kinetic framework, representing solute transfer from solid to fluid through convective and diffusive mechanisms. It assumes a constant effective diffusivity, but extensions have incorporated variable diffusivity terms to capture changes in CO_2 density and solute concentration over time.

Suryawanshi & Mohanty Suryawanshi and Mohanty [16], Suryawanshi and Mohanty [57](2018, 2019) applied a variable-diffusion Sovová model for *Argemone mexicana* and *Pongamia pinnata* seeds, obtaining high predictive accuracy (AARD < 5%). Similarly, Wang et al. (2019) and Maitusong et al. (2021) observed that extraction kinetics fitted well to broken-intact cell and shrinking-core models, validating the transition between diffusion-limited and equilibrium stages.

In some cases, two-parameter exponential models or second-order kinetic models have been used for simplicity, especially in rapid-screening studies (e.g., Minaei et al., 2026 for coriander oil). These models accurately describe the biphasic extraction curve, offering easy estimation of equilibrium yield ($Y\infty$) and rate constants (k_1, k_2).

5.3. Thermodynamic Models: Equation of State (Peng–Robinson, Soave–Redlich–Kwong)

Thermodynamic modeling using Equations of State (EOS) is essential for describing phase behavior and predicting solubility over broad temperature-pressure ranges. The Peng–Robinson (PR) and Soave–Redlich–Kwong (SRK) equations are most commonly applied due to their robustness for non-polar and slightly polar mixtures like triglycerides and CO_2.

Studies on *Hemp* (Devi & Khanam, 2019) and *Carrot* (Priyanka & Khanam, 2020) showed that the PR-EOS accurately predicted phase equilibria and the onset of the retrograde solubility phenomenon—a decline in solubility with increasing temperature at constant pressure. Moreover, EOS models assist in estimating critical enhancement regions, guiding optimal temperature and pressure selection for maximum solvating power while avoiding density drops near the pseudo-critical point.

5.4. Simulation of Process Optimization Using Aspen Plus, MATLAB, and COMSOL

With the growing emphasis on process integration and scale-up, numerical simulation tools such as Aspen Plus, MATLAB, and COMSOL Multiphysics are increasingly used to complement experimental optimization.

- Aspen Plus is applied for process flow modeling and energy analysis. It enables the integration of EOS thermodynamic packages (Peng–Robinson or SRK) with SC-CO_2 unit operations, allowing evaluation of solvent recycling, heat exchanger duties, and compressor energy requirements. Minaei et al. (2026) implemented such simulation for coriander seed oil extraction, achieving 32% energy efficiency and identifying the liquid-CO_2 pump as the major source of exergy loss (≈ 42%).
- MATLAB is used for data fitting and optimization of kinetic and statistical models. Studies by Rai et al. (2017) and Suryawanshi & Mohanty (2018) employed MATLAB's global optimization routines (Box–complex and Levenberg–Marquardt algorithms) to fit the Sovová model, achieving high correlation ($R^2 > 0.98$) and minimal RMSE (< 0.004).
- COMSOL Multiphysics supports CFD-based simulations of fluid flow and diffusion within packed extraction beds. Though still limited in SC-CO_2 seed-oil applications, preliminary studies demonstrate its potential to visualize pressure gradients, temperature fields, and channeling effects in large-scale extractors.

6. Summary of Parameter Effects on SC-CO_2 Extraction of Seed Oils

The performance of supercritical CO_2 (SC-CO_2) extraction depends on the intricate balance among its operating parameters—pressure, temperature, particle size, extraction time, and co-solvent ratio. Each factor influences the thermodynamic equilibrium, solvent density, and mass-transfer kinetics that govern extraction yield and selectivity as shown in Figure 1.

At the core of optimization lies the interplay between pressure and temperature. Increasing pressure generally enhances CO_2 density and solvating power, resulting in higher extraction yields up to a saturation point, beyond which further compression yields diminishing returns. In contrast, temperature exhibits dual effects: at low pressure it enhances vapor pressure and solute diffusivity, but at high pressure it can decrease solvent density—leading to the retrograde solubility phenomenon.

Particle size and bed packing density control internal diffusion and flow uniformity. Smaller particles shorten diffusion paths, accelerating extraction rates, but excessive size reduction can cause channeling and pressure drop, reducing mass-transfer efficiency. Extraction time affects the transition from the solubility-controlled to the diffusion-controlled regime; most systems reach equilibrium within 60–150 min.

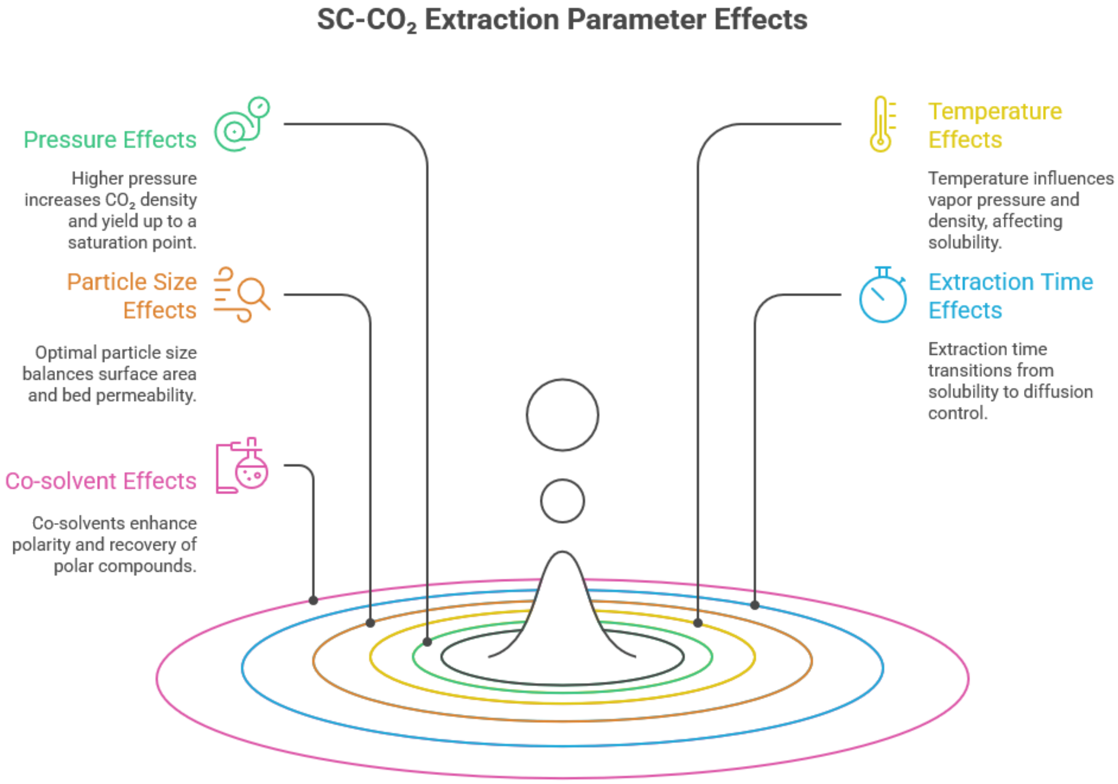


Figure 1. Summary of Parameter Effects on SC-CO_2 Extraction of Seed Oils

The addition of co-solvents (typically ethanol 5–10%) modulates solvent polarity, improving recovery of moderately polar compounds such as phenolics and sterols. However, excessive co-solvent (> 20%) can reduce selectivity and complicate solvent separation. Integration of these parameters through multivariate optimization (RSM, ANN, or hybrid models) allows the design of energy-efficient, selective, and reproducible SC-CO_2 processes tailored for diverse seed matrices. Table 7 summarizes the key process parameters that influence SC-CO_2 extraction of seed oils.

Table 7. Summary of Major Process Parameters Influencing SC-CO_2 Extraction of Seed Oils

Parameter	Typical Range	Observed Trend	Mechanistic Effect
Pressure	10–45 MPa (100–450 bar)	Yield increases with pressure due to higher CO_2 density; plateaus beyond 35 MPa	Enhances solute solubility and solvent loading; high pressure compresses CO_2 molecules, improving mass transfer
Temperature	35–80 °C	Complex: positive at low pressure; negative at high pressure (retrograde)	Competes between increased vapor pressure (↑ solubility) and reduced density (↓ solubility); influences extract composition
CO_2 Flow Rate	5–25 g min^{-1}	Moderate increase in yield up to optimum; excessive flow gives poor	Determines residence time and solvent–solute equilibrium; too high flow causes incomplete saturation

Parameter	Typical Range	Observed Trend	Mechanistic Effect
		solvent–solute contact	
Particle Size	0.15–1.0 mm	Medium size (~0.5–0.7 mm) gives maximum yield; too small causes bed compaction	Balances surface area and bed permeability; small particles increase diffusion but raise pressure drop
Extraction Time	30–180 min	Rapid yield increase in first hour; equilibrium after ~90 min	Two-stage kinetic profile: solubility-controlled phase followed by diffusion-limited regime
Co-solvent Type & Ratio	Ethanol or MeOH/EtOH (0–20% v/v)	Moderate (5–10%) enhances yield; > 20% may reduce selectivity	Increases solvent polarity, extracts phenolics, sterols, tocopherols; excessive addition alters phase behavior
Bed Packing Density	0.3–0.6 g cm^{-3}	Denser beds reduce flow uniformity; loose packing decreases contact	Affects CO_2 distribution, residence time, and axial dispersion; impacts diffusion resistance

7. Future Trends and Research Opportunities

Future research in supercritical CO_2 (SC-CO_2) extraction of seed oils is expected to advance toward greener solvents, integrated processes, and intelligent optimization frameworks. The development of eco-friendly co-solvents, such as natural deep eutectic solvents (NaDES) or bio-based modifiers (e.g., ethyl lactate, glycerol), offers new possibilities for tuning solvent polarity and enhancing selectivity without compromising recyclability. Combining SC-CO_2 with ionic liquids or lipidic co-solvents may enable selective recovery of phenolics, tocopherols, and sterols while maintaining process sustainability. These innovations will require rigorous assessment of phase behavior, solvent regeneration, and toxicity to ensure environmental and industrial feasibility.

A second emerging direction lies in multi-objective and energy-integrated optimization. Traditional single-factor optimization has evolved into hybrid frameworks that couple Response Surface Methodology (RSM) with Artificial Neural Networks (ANN) or Genetic Algorithms (GA) for simultaneous maximization of yield, bioactive content, and energy efficiency. Studies such as those by Minaei et al. (2026) demonstrated that integrating energy–exergy (2E) analyses into optimization reveals hidden inefficiencies, such as pump irreversibility and compressor energy loss. Future SC-CO_2 systems are expected to feature real-time adaptive control, using AI-assisted algorithms to adjust process parameters dynamically based on feedback from sensors and predictive models.

Another key trend is the expansion of modeling and simulation capabilities. Current empirical and semi-empirical models (Chrastil, Sovová) will be enhanced through multiscale computational approaches combining thermodynamic equations of state (Peng–Robinson, SRK) with Computational Fluid Dynamics (CFD) and digital-twin environments. Simulation tools such as Aspen Plus, MATLAB, and COMSOL

Multiphysics can be integrated with experimental and sensor data to predict phase behavior, temperature gradients, and diffusion dynamics inside packed extraction beds. This digitalization will support process scale-up and equipment design while reducing experimental workload and enabling virtual prototyping of SC-CO_2 systems.

Finally, the long-term research vision should emphasize sustainability, process intensification, and circular bioeconomy. Hybrid extraction technologies—such as ultrasound- or microwave-assisted SC-CO_2—offer energy savings and higher extraction kinetics, while nano-encapsulation or supercritical anti-solvent (SAS) techniques can enhance the stability and bioavailability of extracted oils. Large-scale implementation will benefit from life-cycle assessment (LCA) and techno-economic analysis (TEA) to quantify environmental impact and guide process design toward carbon neutrality. Establishing open-access databases of solubility and kinetic parameters, coupled with AI-driven data mining, will accelerate innovation and standardize global research efforts. Overall, the future of SC-CO_2 extraction lies in smart, sustainable, and data-driven engineering that unites process optimization, green chemistry, and digital modeling for efficient seed-oil valorization.

The integration of artificial intelligence (AI) and digital-twin technologies represents a promising direction for the next generation of SC-CO_2 extraction systems. AI-driven predictive control and machine learning algorithms can continuously optimize parameters such as pressure, temperature, and flow rate in real time, improving yield consistency and energy efficiency. Meanwhile, digital-twin modeling can simulate extraction dynamics under varying conditions, enabling rapid scenario testing, fault detection, and scale-up validation without costly experimentation. The combination of these tools with existing thermodynamic and kinetic models can bridge the gap between laboratory precision and industrial robustness, making SC-CO_2 extraction a smart, adaptive, and sustainable technology for future bioprocess industries.

8. Conclusion

Supercritical carbon dioxide (SC-CO_2) extraction has emerged as a powerful green technology for recovering high-value seed oils and bioactives with superior purity and functionality. This review has outlined the effects of key parameters—pressure, temperature, extraction time, and co-solvent ratio—on yield, selectivity, and energy efficiency. Modeling approaches such as the Chrastil and Sovová equations, response surface methodology (RSM), and kinetic modeling have been instrumental in describing solubility behavior and optimizing process performance. The integration of machine learning tools such as artificial neural networks (ANN) and hybrid optimization frameworks has further enhanced predictive accuracy and process control.

However, while laboratory-scale studies demonstrate excellent efficiency and selectivity, industrial scalability remains a challenge due to the high initial capital cost of SC-CO_2 systems, energy demand for CO_2 compression, and the need for robust process control under high pressures. The sustainability of large-scale operations requires innovations in energy recovery, CO_2 recycling loops, and modular continuous extraction systems to lower environmental and economic footprints. Future efforts should focus on combining SC-CO_2 with renewable energy inputs and circular bioeconomy strategies to make the technology more accessible, cost-effective, and sustainable for industrial adoption in the food, cosmetic, and pharmaceutical sectors.

Competing Interest

The authors whose names are listed immediately below certify that they have NO affiliations with or involvement in any organization or entity with any financial interest, or non-financial interest in the subject matter or materials discussed in this manuscript.

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Data Availability

The data that support the findings of this study are available from the corresponding author, upon reasonable request

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