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Original Article

Probabilistic Risk Assessment of Pesticide Residues in Coconut (*Cocos nucifera L.*) Water and Pulp Using Bioconcentration Factors, Dietary Intake, and Monte Carlo Simulation

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Abstract

Coconut (*Cocos nucifera L.*) is a nutritionally valuable crop extensively cultivated in tropical regions, with fresh coconut water and pulp being consumed worldwide. However, commercial production frequently relies on pesticides — including abamectin, azoxystrobin, cyproconazole, difenoconazole, dimethoate, imidacloprid, metalaxyl, and thiamethoxam — that may accumulate in these edible matrices, creating potential dietary exposure pathways. This study presents a comprehensive probabilistic assessment of bioconcentration factors (BCFs) and human health risks for eight pesticides (abamectin, azoxystrobin, cyproconazole, difenoconazole, dimethoate, imidacloprid, metalaxyl, and thiamethoxam) in coconut water and pulp. Using Monte Carlo simulations (100,000 iterations per pesticide) that integrate plant physiological parameters, pesticide physicochemical properties, and residue concentrations, we estimated probability distributions for compartment-specific BCFs and daily intakes for adult consumers. Sensitivity analysis using Spearman rank correlations identified the most influential parameters driving risk uncertainty. Based on the 5th percentile margin of safety (MoS_P5) relative to regulatory reference doses (RfD), pesticides were classified into risk categories: cyproconazole (MoS_P5=5.8), difenoconazole (MoS_P5=8.3), and metalaxyl (MoS_P5=4.6) as high risk; dimethoate (MoS_P5=38.1), imidacloprid (MoS_P5=21.3), and thiamethoxam (MoS_P5=81.6) as moderate risk; and abamectin (MoS_P5=142.8) and azoxystrobin (MoS_P5=599.2) as low risk. Sensitivity analysis demonstrated that residue concentrations in the relevant edible matrix and pesticide degradation rate in the plant are the primary determinants of human health risk, while stem-sap partition coefficients showed negligible influence. Compartment-specific analysis revealed that water intake risk is dominated by Cwater and TSCF, while pulp intake risk is dominated by Cpulp and LogKow. These findings indicate that while some pesticides present acceptable safety margins, compounds with prolonged plant half-lives (cyproconazole: 49.3 days; difenoconazole: 73.7 days) warrant regulatory scrutiny. The probabilistic approach identifies risk scenarios potentially overlooked by deterministic assessments, providing a more robust foundation for food safety management in the coconut production chain.

Keywords: Coconut water; coconut pulp; food safety; fungicide; mathematical modelling; pesticide residues.

INTRODUCTION

Coconut (*Cocos nucifera* L.) represents one of the most economically significant perennial crops in tropical and subtropical regions, with global production exceeding 60 million tons annually (FAOSTAT, 2023). The fruit is prized both for its refreshing water, a hypotonic beverage rich in minerals, sugars, and vitamins and its succulent pulp (endosperm), which contains functional lipids, proteins, and dietary fiber (Yingshuang *et al.* 2024; Akpro *et al*., 2019; Prades *et al*., 2012). Fresh coconut consumption has increased substantially worldwide, driven by perceived health benefits and the global expansion of tropical food products (Carvalho *et al*., 2006; Rethinam & Krishnakumar, 2022).

However, intensive coconut cultivation frequently requires pesticide applications to manage pest pressures from insects (e.g., *Rhynchophorus ferrugineus*,

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Aceria guerreronis), fungal pathogens (e.g., *Ganoderma boninense*, *Phytophthora palmivora*), and weeds that reduce productivity (EFSA, 2022). These pesticides may persist through fruit development and accumulate in edible tissues, creating potential dietary exposure pathways to compounds with known or suspected toxicity. Several monitoring studies have documented pesticide residues in coconut products. Ferreira *et al.* (2016) detected multiple pesticides including carbofuran, carbendazim, thiabendazole, cyproconazole, and difenoconazole in coconut water and pulp samples from different Brazilian regions, with some samples showing quantifiable residues below European Union maximum residue limits (MRLs). Similarly, Pandey *et al*. (2010) reported organochlorine pesticide residues in dried coconut products from Indian markets. Pesticide residues were detected in some samples of both FTCW (fresh tender coconut water) and PTCW (packaged tender coconut water) , while heavy metals were detected in all samples collected from all three states of India (Jonnalagadda *et al*., 2022).

The bioconcentration factor (BCF), defined as the equilibrium concentration ratio of a substance between an organism and its exposure medium (Jonsson & Queiroz, 2023; Andreu-Sanchez *et al*., 2012; Bacci, 1993), and provides a mechanistic basis for estimating pesticide accumulation in plants. The concentration value in the tissue at steady-state equilibrium at a given concentration of the pesticide in the medium, calculated using this factor, can be compared with the MRL value of the food product (fruit). This concentration allows calculating the maximum intake of the pesticide through consumption of the food product so that the reference dose (RfD) is not exceeded. This dose is an estimate of the maximum daily oral exposure to a chemical substance that is likely to be without an appreciable risk of deleterious effects over a human lifetime (Paraíba *et al.*, 2025; Jonsson *et al.*, 2019).

For fruit crops, BCF enables prediction of pesticide residues in harvested products based on environmental concentrations, supporting dietary exposure assessments and the establishment of safe application practices (Trapp *et al*., 2003; Paraiba, 2007). Paraiba (2007) developed a deterministic model for pesticide bioconcentration in fruit trees that integrates plant physiological parameters (transpiration rate, biomass, and growth dilution) with pesticide physicochemical properties (octanol-water partition coefficient, degradation kinetics, xylem transport efficiency).

Despite its utility, deterministic BCF modelling presents inherent limitations. Plant physiological parameters exhibit substantial variability due to environmental conditions, cultivar differences, and phenological stage. Pesticide properties determined under laboratory conditions may not reflect field behaviour, and degradation rates vary with temperature, radiation, and plant metabolic activity (Fantke *et al.,* 2014). Furthermore, concentrations in edible tissues depend on partitioning dynamics between fruit compartments (water, pulp) that are influenced by lipid content and compound lipophilicity. Deterministic point estimates cannot adequately capture these multiple sources of variability and uncertainty, potentially leading to risk classifications that are either overprotective or underprotective of public health.

Probabilistic approaches, particularly Monte Carlo simulation, offer a rigorous framework for addressing parametric uncertainty in environmental and human health risk assessments (US-EPA, 2014). By representing uncertain input parameters as probability distributions and repeatedly sampling from these distributions, Monte Carlo methods generate empirical distributions of model outputs (e.g., BCF, daily intake) that reflect the combined effects of all sources of variability. This approach enables risk managers to evaluate the likelihood of exceeding safety thresholds rather than relying on single-point comparisons (Kroese *et al*., 2011). Spearman rank correlation analysis further allows identification of parameters contributing most to output uncertainty, guiding prioritization of data collection and model refinement efforts (Saltelli *et al.,* 2004).

The present study advances previous work by: adapting the Paraiba (2007) model specifically for coconut palms with compartment-specific BCF estimation for water and pulp; incorporating probability distributions for all key input parameters based on published data; conducting comprehensive uncertainty and sensitivity analysis using Monte Carlo simulation (100,000 iterations per pesticide); classifying dietary risk using the 5th percentile margin of safety (MoS_P5) relative to regulatory reference doses; and performing compartment-specific sensitivity analysis to identify critical parameters for water versus pulp consumption scenarios. We hypothesize that probabilistic assessment will reveal risk scenarios not captured by deterministic analyses, providing more scientifically defensible foundations for food safety management in the coconut production chain.

MATERIALS AND METHODS

Conceptual Framework and Mathematical Model

The bioconcentration factor for pesticides in whole coconut fruit $BCF_{coconut}$ (L kg^{-1}) was adapted from the fruit tree model developed by Paraiba (2007), which describes steady-state partitioning between xylem transport, phloem translocation, metabolic degradation, and growth dilution:

$$BCF_{coconut} = \frac{Q_x Q_f TSCF}{Q_x + K_p K_{stem\_sap} M} \quad (1)$$

where Q_x 100 L d^{-1} is average daily sap flow rate in xylem, Q_f = 6.22 L kg^{-1} is volume of elaborated sap required to produce 1 kg fresh coconut over approximately 180 days, *TSCF* (dimensionless) is the transpiration stream concentration factor, K_p (d^{-1}) is first-order pesticide degradation rate in plant tissues, K_{stem_sap} (L kg^{-1}) is pesticide partition coefficient between stem tissue and sap, and M = 500 kg is the total fresh mass of the coconut palm.

This formulation assumes that pesticide uptake occurs primarily via transpiration-driven mass flow, with subsequent partitioning between aqueous (sap) and solid (stem, fruit) phases. Importantly, $BCF_{coconut}$ is independent of application rate or method, being determined solely by plant physiology and pesticide properties.

The pesticide pulp-water partition coefficient (K_{pulp_water}) was estimated using a lipid-normalized linear model (Trapp *et al.*, 2001; Briggs, 1981):

$$K_{pulp\_water} = f_{lipid} K_{ow} \quad (2)$$

where f_{lipid} = 0.33 is the volumetric lipid fraction of coconut pulp and $K_{ow} = 10^{\log Kow}$ is the pesticide octanol-water partition coefficient.

Assuming equilibrium and mass balance, the compartment-specific bioconcentration factors (L kg^{-1} fresh tissue) are (original mass-balance derivations for coconut, this study):

$$BCF_{water} = \frac{m_{coconut} BCF_{coconut}}{\rho_{water} v_{water} + m_{pulp} K_{pulp\_water}} \quad (3)$$

$$BCF_{water} = \frac{m_{coconut} BCF_{coconut} K_{pulp\_water}}{\rho_{water} v_{water} + m_{pulp} K_{pulp\_water}} \quad (4)$$

where BCF_{water} (L kg^{-1}) is the bioconcentration factor of the pesticide in the water, BCF_{pulp} (L kg^{-1}) is the bioconcentration factor of the pesticide in the pulp, $m_{coconut}$ = 0.55 kg is total coconut mass, m_{pulp} = 0.10 kg is the total pulp mass, V_w = 0.45 L is the total water coconut, and ϱ_w = 1.01 kg/L is the coconut water density.

Dietary Intake and Risk Characterization

Daily pesticide intake from consuming one fresh coconut was calculated for a 70 kg adult:

$$DI_{total} = \frac{\rho_{water} V_w BCF_{water} C_{water}}{70} + \frac{m_{pulp} BCF_{pulp} C_{pulp}}{\rho_{pulp} 70} \quad (5)$$

where DI_{total} is daily total intake (mg kg^{-1} pc), C_{water} (mg L^{-1}) is the concentration of the pesticide in the water, C_{pulp} (mgkg^{-1}) is the concentration of the pesticide in the pulp, and $\varrho_{pulp} \approx 1.08$ kg/L is the pulp density. Compartment-specific daily intakes DI_{water} and DI_{pulp} were calculated analogously.

The daily intake of the pesticide from the coconut water, DI_{water}, and the daily intake of the pesticide from the coconut pulp, DI_{pulp}, for an adult with a body weight of 70 kg was calculated using, respectively:

$$DI_{water} = \frac{\rho_{water} V_w BCF_{water} C_{water}}{70} \quad (6)$$

and

$$DI_{pulp} = \frac{m_{pulp} BCF_{pulp} C_{pulp}}{\rho_{pulp} 70} \quad (7).$$

The margin of safety (MoS) was defined as the ratio of the reference dose (RfD) established by regulatory agencies to the estimated daily intake (DI), so that higher MoS values indicate lower risk:

$$MoS = \frac{RfD}{DI} \quad (8)$$

where MoS (dimensionless) is the margin of safety, RfD (mg kg^{-1} body weight day^{-1}) is the regulatory reference dose, and DI (mg kg^{-1} body weight day^{-1}) is the estimated daily intake.

A summary of all model symbols and units used in Equations (1)–(8) is provided below: Q_x (L day^{-1}) = xylem sap flow rate; Q_f (L kg^{-1}) = elaborated sap volume per kg coconut; *TSCF* (dimensionless) = transpiration stream concentration factor; K_p (day^{-1}) = first-order pesticide degradation rate in plant; K_{stem_sap} (L kg^{-1}) = stem–sap partition coefficient; M (kg) = total palm mass; f_{lipid} (dimensionless) = pulp lipid fraction; Kow (dimensionless) = octanol–water partition coefficient; mcoconut (kg) = total coconut mass; mpulp (kg) = pulp mass; V_w (L) = coconut water volume; ρ_w (kg L^{-1}) = coconut water density; ρ_{pulp} (kg L^{-1}) = pulp density; C_{water} (mg L^{-1}) = pesticide concentration in sap phase supplying coconut water; C_{pulp} (mg kg^{-1}) = pesticide concentration in sap phase supplying pulp.

Based on the 5th percentile of the simulated MoS distribution (MoS_P5), pesticides were classified into four risk categories: MoS_P5 < 1 (unacceptable risk), 1 ≤ MoS_P5 < 10 (high risk), 10 ≤ MoS_P5 < 100 (moderate risk), and MoS_P5 ≥ 100 (low risk).

Input Parameters and Probability Distributions

Pesticide Physicochemical Properties

The logarithm of the octanol-water partition coefficient (*LogKow*) for each pesticide was obtained from PubChem and the Pesticide Properties Database (PPDB). Values ranged from highly hydrophilic (thiamethoxam: *LogKow* = -0.13) to highly lipophilic (abamectin and difenoconazole: *LogKow* = 4.4) (Table 1).

The logarithm of the pesticide octanol-water partition coefficient, *LogKow*, was modelled using a normal distribution *LogKow.N* ($\mu_{LogKow,}$ σ^2_{LogKow}), with the mean (μ_{LogKow}) and standard deviation (σ^2_{LogKow}) obtained from PubChem (https://pubchem.ncbi.nlm.nih.gov/) and the Pesticide Properties Database (PPDB) (https://sitem.herts.ac.uk/aeru/ppdb/en/). Full distribution parameters (type, mean, SD/CV, unit, and source) for all Monte Carlo input variables are provided in Supplementary Table S1.

Table 1. Physicochemical properties, toxicological reference values, and input parameters for the eight studied pesticides.

Pesticide	$LogK_{ow}$	RfD (mg $kg^{-1}day^{-1}$)	MRL (mg kg^{-1})	TSCF mean	Half-life mean (day)	K_p mean (day^{-1})	K_{stem_sap} mean (L kg^{-1})
Abamectin	4.4	.0005	.01	.191	2.26	.0593	208.46
Azoxystrobin	2.5	.1	.05	.744	8.67	.0253	177.47
Cyproconazole	2.9	.01	.3	.701	9.30	.0147	157.35
Difenoconazole	4.4	.01	.5	.191	3.72	.0098	159.20
Dimethoate	0.7	.002	.02	.220	.88	.2520	6.43
Imidacloprid	0.57	.06	.5	.183	1.73	.0117	41.68
Metalaxyl	1.75	.08		.602	8.47	.0393	29.15
Thiamethoxam	-0.13	.005	.02	.055	3.03	.0219	10.16

Note: RfD: reference dose (mg kg^{-1} body weight day^{-1}); MRL: maximum residue limit (mg kg^{-1}); TSCF: transpiration stream concentration factor; Kstem_sap: stem-sap partition coefficient (L kg^{-1}).

The transpiration stream concentration factor (*TSCF*), which quantifies the efficiency of pesticide uptake into xylem sap, was estimated using the Gaussian model of Trapp (2004):

$$TSCF = a \times exp\left[-\frac{(LogKow-b)^2}{c}\right] \qquad (9)$$

with parameters a = 0.756, b = 2.50, c = 2.58. *TSCF* values were simulated with variability reflecting the uncertainty in the Trapp model parameters (coefficient of variation = 7%). Mean *TSCF* values ranged from 0.055 (thiamethoxam) to 0.744 (azoxystrobin) (Table 1). Because TSCF is derived from LogKow via Equation (9), the two are not independent in the sensitivity analysis. The Spearman coefficient for TSCF captures both the LogKow-driven component and additional uncertainty in the Trapp model parameters (CV = 7%). Readers should therefore interpret the LogKow and TSCF rows in Table 4 as partially overlapping sources of variance rather than independent contributions.

Plant Physiological Parameters

Xylem sap flow rate (Q_s) for a mature coconut palm under high evaporative demand was fixed at 100 L/day based on empirical measurements by Passos *et al.* (2019) and Carr (2011). The volume of elaborated sap required to produce 1 kg fresh coconut was estimated at 6.22 L kg^{-1} based on inflorescence sap production rates reported by Novarianto *et al.* (2021). Total fresh mass of a productive 8-year-old coconut palm (M) was set at 500 kg (Chan & Elevitch, 2006; Kumar & Balakrishna, 2009). Pulp lipid fraction (f_{lipid}) was set at 0.33 (Dayrit, 2024). These physiological parameters were treated as fixed constants for three reasons: (i) published measurements for mature Tall-variety coconut palms under comparable tropical conditions are highly consistent (CV < 10% across studies; Passos *et al.*, 2019; Carr, 2011); (ii) preliminary sensitivity runs showed that their individual and joint contribution to output variance was below 5%, dominated by the stochastic parameters LogKow, Kp, and residue concentrations; and (iii) fixing them keeps the model parsimonious and focused on the dominant sources of uncertainty. Nevertheless, we acknowledge that these values may differ with cultivar, palm age, fruit maturity stage, and water deficit conditions.

Pesticide Fate Parameters

In the computational model, the pesticide degradation rate in the plant (*Kp*) is derived directly from the plant half-life. For each pesticide, the plant half-life t½ was modelled as lognormally distributed, with the mean equal to the pesticide-specific value reported in Table 1 and a fixed standard deviation of 6 days representing intra-species variability in plant metabolic activity (Fantke et al., 2014). No generic 30-day distribution was used. Dimethoate (t½ = 2.88 d) and metalaxyl (t½ = 18.47 d) half-lives were taken from Fantke *et al.* (2014); cyproconazole (t½ = 49.30 d) and difenoconazole (t½ = 73.72 d) from Juraske *et al*. (2008); abamectin (t½ = 12.26 d), azoxystrobin (t½ = 28.67 d), imidacloprid (t½ = 61.73 d), and thiamethoxam (t½ = 33.03 d) from primary field dissipation studies cited in Table 1. This lognormal parameterisation ensures only positive values are sampled and captures inherent variability in plant degradation processes without relying on empirical soil–plant transfer relationships.

Plant degradation half-lives (t½) were obtained from experimental data, with mean values ranging from 2.88 days (dimethoate) to 73.72 days (difenoconazole) (Table 1). Stem-sap pesticide partition coefficients (K_{stemp_sap}) were obtained from Paraíba *et al.* (2022), ranging from 6.43 L kg^{-1} (dimethoate) to 208.46 L kg^{-1} (abamectin). The daily degradation rate of each pesticide in the coconut palm, K_p (1/day), was estimated from the pesticide's half-life in the plant, t½. It was assumed that t½ follows a pesticide-specific lognormal distribution with SD = 6 days, ensuring that only positive values are sampled. The degradation rate for first-order kinetics was estimated by $K_p = \frac{ln2}{t_{1/2}}$. The lognormal distribution of was modelled by $t_{1/2}.LogNormal\ (\mu_{log}, \sigma^2_{log})$.

The partition coefficients of pesticides between the stem and sap, K_{stemp_sap}, were based on the pesticides from the experimental work of Paraíba *et al* (2022). A normal distribution with appropriate mean and standard deviation was used. For the K_{stemp_sap} of the fungicide difenoconazole, the value was estimated by $LogK_{stipe\_sap} = 1.144 + 0.299\ LogKow - 0.219LogSol$, resulting in $K_{stemp\_sap} = 159.2$ (Paraiba *et al*., 2022).

Residue Concentrations

Concentrations in coconut water (C_{water}) and pulp (C_{pulp}) at harvest were modelled as lognormally distributed with means equal to the Maximum Residue Limit (MRL) for each pesticide on tropical fruits (US-EPA or EFSA) and a coefficient of variation CV = 0.5. It is important to note that C_{water} and C_{pulp} represent pesticide concentrations in the sap phase supplying each fruit compartment, not final tissue concentrations at harvest; MRL values aren used as conservative upper-bound analogues of maximum field sap concentrations. BCF_{water} and BCF_{pulp} (Equations 3 and 4) then partition these sap-phase concentrations into each edible compartment, so no double-counting of the bioconcentration process occurs. This approach follows regulatory guidelines for screening-level exposure assessment, representing a conservative assumption that residues may approach legal limits in some production scenarios (Codex Alimentarius, EFSA, EPA).

Monte Carlo Simulation Protocol

Simulations were implemented in Python 3.9 using NumPy, SciPy, and Pandas libraries. For each of eight pesticides, we performed 100,000 iterations with Latin Hypercube sampling to ensure efficient coverage of input distributions.

Per iteration: Sample *LogKow* from normal distribution (parameters from databases); Sample *TSCF* model parameters and calculate *TSCF* using Equation (9); Sample plant half-life from lognormal distribution and calculate $K_p = \frac{ln2}{t_{1/2}}$; Sample K_{stem_sap} from normal distribution; Sample C_{water} and C_{pulp} from lognormal distributions (mean = MRL, CV = 0.5); Calculate $BCF_{coconut}$ using Equation (1); Calculate $K_{pulp\_water} = f_{lipid} \times 10^{LogKow}$ using Equation (2); Calculate BCF_{water} and BCF_{pulp} using Equations (3) and (4); Calculate DI_{total}, DI_{water}, and DI_{pulp} using Equations (5)-(7); Calculate MoS_{total}, MoS_{water}, MoS_{pulp} using Equation (8). Convergence was assessed by monitoring the stability of 5th and 95th percentiles for key outputs; all metrics stabilized within 50,000 iterations.

Sensitivity Analysis

Spearman rank correlation coefficients were calculated between each input parameter (*LogKow, TSCF,* K_p, K_{stem_sap}, C_{water}, C_{pulp}) and model outputs (DI_{total}, DI_{water}, DI_{pulp}) using the 100,000 simulated values per pesticide. Parameters with $|\rho|$ >0.5 were considered highly influential; 0.3< $|\rho|$ <0.5 moderately influential; and $|\rho|$ <0.3 weakly influential.

Spearman rank correlation coefficients were calculated between each input parameter (*LogKow, TSCF, Kp, Kstem_sap, Cwater, Cpulp*) and model outputs (*BCFs, DIs, MoS*) using the 100,000 simulated values per pesticide. Spearman's ρ measures monotonic association without assuming linearity, making it appropriate for the non-linear relationships inherent in the bioconcentration model. Parameters with $|\rho|$ >0.5 were considered highly influential; 0.3< $|\rho|$ <0.5 moderately influential; and $|\rho|$ <0.3 weakly influential. Compartment-specific sensitivity analyses were performed for DI_{water} and DI_{pulp} to identify parameters driving risk in each consumption scenario.

Model Limitations and Assumptions

Key limitations include: equilibrium partitioning assumption between water and pulp at harvest may not reflect kinetic limitations; generic TSCF model developed primarily for herbaceous crops; fixed plant physiological parameters that may vary with cultivar, age, and environment; no compartment-specific metabolism; and MRL-based concentrations representing conservative screening-level estimates rather than typical exposures. Fixed plant physiological parameters (Q_x, Q_f, M, f_{lipid}) may underestimate total model uncertainty for cultivars or environmental conditions that deviate substantially from the values adopted here. These limitations imply that risk classifications should be interpreted as screening-level indicators rather than definitive regulatory determinations.

RESULTS

Bioconcentration Factors

Table 1 presents the physicochemical properties, toxicological reference values, and input parameters for the eight pesticides studied. *LogKow* values ranged from highly hydrophilic (thiamethoxam: -0.13) to highly lipophilic (abamectin and difenoconazole: 4.4). Plant half-lives varied substantially, from 2.9 days (dimethoate) to 73.7 days (difenoconazole). *TSCF* values were highest for compounds with *LogKow* near the optimum of 2.5 (azoxystrobin: 0.74; cyproconazole: 0.70; metalaxyl: 0.60).

Estimated bioconcentration factors varied substantially among pesticides and across fruit compartments (Table 2). Metalaxyl exhibited the highest mean *BCF* for whole coconut (0.595 L kg^{-1}) and pulp (2.63 L kg^{-1}), reflecting its moderate lipophilicity (*LogKow* = 1.75) and relatively slow degradation (half-life 18.5 days). Cyproconazole also showed high pulp accumulation (BCF_{pulp} = 2.02 L kg^{-1}) due to its longer half-life (49.3 days). In contrast, abamectin showed the lowest BCF_{water} (1.46×10^{-5} L kg^{-1}), despite its high lipophilicity (*LogKow* = 4.4), due to rapid degradation (half-life 12.3 days) and strong stem partitioning (K_{stem_sap} = 208.5 L kg^{-1}).

Table 2. Bioconcentration factors (*BCF*) for coconut water and pulp.

Pesticide	BCF_{water} mean (L kg^{-1})	BCF_{water} P5_P95	BCF_{pulp} mean (L kg^{-1})	BCF_{pulp} P5_P95	BCF_{pulp}/BCF_{water} Ratio
Abamectin	1.46×10^{-5}	(4.9×10^{-6} - 3.1×10^{-5})	0.114	(0.049 - 0.210)	7,800
Azoxystrobin	0.0111	(0.0056 - 0.0190)	1.13	(0.66 - 1.76)	102
Cyproconazole	0.00797	(0.0039 - 0.0139)	2.02	(1.19 - 3.13)	254
Difenoconazole	1.02×10^{-4}	(3.5×10^{-5} - 2.1×10^{-4})	0.796	(0.357 - 1.42)	7,800
Dimethoate	0.143	(0.068 - 0.247)	0.246	(0.095 - 0.479)	1.7
Imidacloprid	0.329	(0.161 - 0.553)	0.423	(0.163 - 0.816)	1.3
Metalaxyl	0.142	(0.080 - 0.225)	2.63	(1.51 - 4.09)	18.5
Thiamethoxam	0.193	(0.075 - 0.366)	0.0505	(0.0149 - 0.111)	0.26

Note: Values represent means with 5th-95th percentile ranges in parentheses from Monte Carlo simulations (100,000 iterations). The pulp/water ratio illustrates the effect of lipophilicity on partitioning.

Table 2 presents the estimated bioconcentration factors for coconut water and pulp. Lipophilic compounds (*LogKow*>3) showed extreme partitioning into pulp, with BCF_{pulp}/BCF_{water} ratios of approximately 7,800 for abamectin and difenoconazole. Moderately lipophilic compounds (*LogKow* 1.75-2.9) showed ratios of 18-254, while hydrophilic compounds (*LogKow*<1) showed comparable or higher BCF_{water} values relative to pulp. Thiamethoxam (*LogKow* = -0.13) exhibited BCF_{water} nearly four-fold higher than BCF_{pulp}.

Daily Intake and Risk Classification

Estimated daily intakes and margins of safety are presented in Table 3. Mean DI_{total}values ranged from 1.51 $\times 10^{-6}$ mg kg^{-1} day^{-1} (abamectin) to 8.78×10^{-3} mg $kg^{-1}day^{-1}$ (metalaxyl). Based on MoS_P5, three pesticides were classified as high risk: cyproconazole (5.8), difenoconazole (8.3), and metalaxyl (4.6). Four pesticides were classified as moderate risk: dimethoate (38.1), imidacloprid (21.3), and thiamethoxam (81.6). Abamectin (MoS_P5=142.8) and azoxystrobin (599.2) were classified as low risk. A comparison between deterministic (mean-parameter) and probabilistic (MoS_P5) risk classifications is presented in Table 5, illustrating that all pesticides appear acceptable under the deterministic approach (mean MoS > 10 for all compounds), whereas the probabilistic approach identifies cyproconazole, difenoconazole, and metalaxyl as high risk

Table 3. Estimated daily intake (*DI*), margin of safety (MoS), and risk classification by compartment.

Pesticide	DI_{total} mean ($mg\ kg^{-1} d^{-1}$)	DI_{total} P95	MoS_{total}_P5	MoS_{water}_P5	MoS_{pulp}_P5	Risk (water)	Risk (pulp)	Risk (total)
Abamectin	1.51×10^{-6}	3.50×10^{-6}	143	211,941	143	Low	Low	Low
Azoxystrobin	7.83×10^{-5}	1.67×10^{-4}	599	12,456	617	Low	Low	Low
Cyproconazole	8.19×10^{-4}	1.73×10^{-3}	5.8	286	5.8	Low	High	High
Difenoconazole	5.25×10^{-4}	1.20×10^{-3}	8.3	12,187	8.3	Low	High	High
Dimethoate	2.49×10^{-5}	5.25×10^{-5}	38	48	127	Moderate	Low	Moderate
Imidacloprid	1.34×10^{-3}	2.82×10^{-3}	21	25	89	Moderate	Moderate	Moderate
Metalaxyl	8.78×10^{-3}	1.74×10^{-2}	4.6	20	5.3	Moderate	High	High
Thiamethoxam	2.61×10^{-5}	6.13×10^{-5}	82	85	1,441	Moderate	Low	Moderate

Note: Classification based on 5th percentile MoS: MoS_P5 ≥ 100 = low risk; 10-100 = moderate risk; 1-10 = high risk; <1 = unacceptable risk.

Plant degradation half-lives ($t_{½}$, days) were obtained from experimental data, with the corresponding first-order degradation rate calculated as $Kp = \ln(2)/t_{½}$. Stem-sap partition coefficients (K_{stem_sap}) were obtained from Paraiba *et al.* (2022). Concentrations in coconut water and pulp were modelled as lognormally distributed with means equal to the Maximum Residue Limit (MRL) for each pesticide on tropical fruits (US-EPA or EFSA) and coefficient of variation CV = 0.5.

Sensitivity Analysis

Table 4 presents Spearman correlation coefficients between input parameters and total daily intake. Residue concentrations emerged as the most influential parameters, with C_{pulp} dominating for lipophilic compounds (ρ = 0.72 to 0.83) and C_{water} dominating for hydrophilic compounds (ρ = 0.60 to 0.66). The degradation rate (K_p) showed consistent negative correlation (ρ = -0.5 to -0.4) for most pesticides, indicating that faster degradation reduces intake. *TSCF* was highly influential for compounds with intermediate *LogKow* (dimethoate, imidacloprid, thiamethoxam; ρ = 0.54 to 0.68). Stem-sap partition coefficients (K_{stem_sap}) showed negligible influence for all pesticides ($|\rho| < 0.1$). Compartment-specific Spearman coefficients for DIwater and DIpulp separately are reported in Supplementary Table S2.

Table 4. Sensitivity analysis - Spearman rank correlation coefficients between input parameters and total daily intake (DI_{total}).

Pesticide	$LogK_{ow}$	*TSCF*	K_p	K_{stem_sap}	C_{water}	C_{pulp}
Abamectin	-0.22	0.48	-0.44	-0.07	0.00	**0.72**
Azoxystrobin	-0.01	0.13	**-0.52**	-0.09	0.04	**0.82**
Cyproconazole	-0.05	0.17	-0.48	-0.08	0.02	**0.83**
Difenoconazole	-0.23	0.49	-0.40	-0.07	0.01	**0.73**
Dimethoate	0.24	**0.54**	-0.47	-0.08	**0.60**	0.23
Imidacloprid	0.26	**0.58**	-0.37	-0.07	**0.65**	0.18
Metalaxyl	0.10	0.27	**-0.51**	-0.08	0.21	**0.74**
Thiamethoxam	0.30	**0.68**	-0.22	-0.03	**0.66**	0.03

Note: Values in bold ($|\rho| > 0.5$) indicate high influence. K_p (degradation rate) shows a negative correlation, indicating that faster degradation reduces intake.

Table 5. Comparison of deterministic (mean-parameter) and probabilistic (MoS_P5) risk classifications for the eight pesticides studied.

Pesticide	Mean MoS (deterministic)	MoS_P5 (probabilistic)	Risk category (deterministic)	Risk category (probabilistic)
Abamectin	1,985	142.8	Low	Low
Azoxystrobin	4,000	599.2	Low	Low
Cyproconazole	51.8	5.8	Moderate	High
Difenoconazole	73.9	8.3	Moderate	High
Dimethoate	338	38.1	Low	Moderate
Imidacloprid	190	21.3	Low	Moderate
Metalaxyl	46.0	4.6	Moderate	High
Thiamethoxam	731	81.6	Low	Moderate

Note: Deterministic mean MoS was calculated using mean values of all input parameters. Risk categories: Low (MoS ≥ 100); Moderate (10 ≤ MoS < 100); High (1 ≤ MoS < 10); Unacceptable (MoS < 1).

DISCUSSION

Probabilistic vs. Deterministic Risk Assessment

The results strongly confirm our hypothesis that probabilistic assessment reveals risk scenarios potentially overlooked by deterministic approaches. While mean daily intakes for all pesticides appear low relative to RfD values, the 5th percentile MoS indicates that in 5% of plausible parameter combinations, intake approaches or exceeds safe levels for cyproconazole, difenoconazole, and metalaxyl. A deterministic analysis using mean parameter values would classify all pesticides as acceptable (mean MoS > 10 for all compounds), potentially underestimating population-level risk.

This divergence between mean and lower-tail estimates arises from the multiplicative nature of uncertainty in the BCF model. When multiple input parameters simultaneously assume values that increase predicted intake (e.g., longer half-life, higher TSCF, higher residue concentrations), the resulting intake can exceed the product of individual mean effects. Probabilistic methods explicitly account for such joint probabilities, providing risk managers with information on the likelihood of exceeding thresholds rather than simple pass/fail determinations.

Determinants of Pesticide Risk in Coconut

Sensitivity analysis identifies pesticide degradation rate in the plant (*Kp*) as a primary factor controlling human health risk. The consistent negative correlation of *Kp* with DI_{total} (ρ = -0.5 to -0.4) across multiple pesticides indicates that faster degradation reliably reduces estimated intake. This finding has practical implications: pre-harvest intervals and pesticide selection should prioritize compounds with rapid plant degradation, even if their physicochemical properties would otherwise suggest accumulation potential.

The three high-risk pesticides illustrate this principle: cyproconazole (half-life 49.3 days), difenoconazole (73.7 days), and metalaxyl (18.5 days). Notably, metalaxyl's half-life is shorter than azoxystrobin's (28.7 days), but its higher MRL (2.0 mg kg^{-1} vs. 0.05 mg kg^{-1}) and lower RfD (0.08 vs. 0.1 mg kg^{-1} day^{-1}) result in a higher risk. Thus, risk integrates degradation, use pattern (reflected in MRL), and toxicity.

The compartment-specific analysis reveals that risk pathways differ fundamentally between water and pulp consumption. For lipophilic pesticides, pulp is the critical risk pathway; for hydrophilic pesticides, water dominates. This has implications for consumption patterns, populations consuming only coconut water face different risk profiles than those consuming whole coconut.

A surprising finding is the negligible influence of K_{stem_sap} on all risk metrics ($|\rho| < 0.1$). This suggests that while stem-sap partitioning affects absolute BCF values, its variability does not contribute meaningfully to uncertainty in risk estimates. For future modelling efforts, this parameter could potentially be treated as fixed without substantial loss of predictive power. Compartment-specific sensitivity results for DIwater and DIpulp are provided in Supplementary Table S2.

Comparison with Previous Studies

Our BCF estimates are consistent with the limited available data on pesticide residues in coconut. Ferreira *et al.* (2016) detected difenoconazole in coconut water samples from Brazil at concentrations below MRL, consistent with our finding that difenoconazole poses high risk primarily through pulp rather than water. Similarly, their detection of cyproconazole in pulp samples aligns with our classification of cyproconazole as high-risk via pulp consumption.

Compared to the deterministic BCF modelling of Paraiba (2007), our probabilistic approach provides additional insight into the range of possible BCF values. BCF values vary by factors of 3-5 between the 5th and 95th percentiles, highlighting the importance of considering variability in regulatory decisions. In the Brazilian regulatory context, maximum residue limits for pesticide residues in fresh coconut are governed by ANVISA Resolução RDC 216/2006 and Instrução Normativa MAPA 42/2008. For cyproconazole and difenoconazole, ANVISA MRLs (0.3 mg kg^{-1} and 0.5 mg kg^{-1}, respectively) align with the EFSA values used in this study. MAPA does not currently list specific MRLs for abamectin or dimethoate in coconut, for which US-EPA limits were therefore applied. Drinking-water quality standards are governed by CONAMA Resolution 357/2005 and Ministry of Health Ordinance GM/MS 888/2021; these instruments do not set pesticide limits specific to coconut water as a fresh fruit product, reinforcing the need for dedicated coconut-specific regulatory guidance in Brazil.

Limitations and Future Research

Several limitations should be acknowledged: the assumption of instantaneous equilibrium between water and pulp may not reflect kinetic limitations during fruit development; the generic *TSCF* model was developed primarily for herbaceous crops and may not fully capture uptake dynamics in woody perennials; physiological parameters were treated as fixed, but actual values vary with cultivar, age, and environment; the model assumes no compartment-specific metabolism; and using MRLs as mean concentrations is a conservative screening-level approach that may overestimate typical exposures.

Future research priorities should include: field studies measuring actual residue concentrations in coconut water and pulp from treated coconut palms; controlled dissipation studies to refine half-life estimates for priority pesticides; investigation of cultivar differences in pesticide uptake and partitioning; and development of coconut-specific *TSCF* relationships. Climate change represents an important source of future uncertainty not captured by the present model. Projected increases in temperature and changes in precipitation patterns in tropical coconut-producing regions may alter xylem sap flow rates, palm water status, and pesticide degradation kinetics in plant tissues, all of which are primary drivers of BCF and dietary intake in our model. Future implementations should therefore incorporate climate projections to assess how shifting environmental conditions may affect pesticide accumulation and human exposure risk in coconut production systems.

CONCLUSION

This study presents a comprehensive probabilistic assessment of pesticide bioconcentration and human health risk for eight pesticides in coconut water and pulp. Key findings include: Risk classification: Based on the 5th percentile margin of safety, cyproconazole (MoS_P5=5.8), difenoconazole (MoS_P5=8.3), and metalaxyl (MoS_P5=4.6) are classified as high risk; dimethoate (38.1), imidacloprid (21.3), and thiamethoxam (81.6) as moderate risk; and abamectin (142.8) and azoxystrobin (599.2) as low risk. These classifications differ from those based on mean values, highlighting the importance of probabilistic approaches.

Compartment-specific risk: For lipophilic pesticides ($LogKow$ > 3), pulp consumption drives risk; for hydrophilic pesticides ($LogKow$ < 1), water consumption is the critical pathway. This has implications for populations with different consumption patterns. Primary risk determinants: Pesticide degradation rate in the plant (Kp) and residue concentrations in edible tissues (C_{pulp} for lipophilic compounds, C_{water} for hydrophilic compounds) are the most influential parameters driving risk uncertainty. Stem-sap partition coefficients (K_{stem_sap}) show negligible influence.

Monitoring priorities: Programs should prioritize direct measurement of residue concentrations in the relevant edible matrix, with secondary attention to characterizing degradation half-lives for compounds with long persistence.Regulatory implications: These findings should be interpreted as screening-level indicators rather than definitive regulatory determinations. In the absence of direct validation against paired field residue data in coconut water and pulp, the model results are best used to prioritise compounds for targeted monitoring and to identify data gaps requiring experimental follow-up. Compounds with plant half-lives exceeding 30 days (cyproconazole, difenoconazole) and those with high MRL-to-RfD ratios (metalaxyl) are flagged as priorities for field dissipation studies and compartment-specific MRL review under tropical conditions.

The probabilistic framework demonstrated here provides a more scientifically defensible foundation for food safety management than deterministic approaches, explicitly accounting for uncertainty and identifying scenarios where risk may be underestimated. Application of this approach to additional pesticides and other fruit crops would enhance the robustness of global food safety systems.

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AUTHOR CONTRIBUTIONS

LCP: Conceptualization, Data curation, Methodology, Writing-Original draft preparation. **CMJ:** Conceptualization, Writing-Reviewing and Editing.

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