Journal of Food Process Engineering

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Journal of Food Process Engineering

ORIGINAL ARTICLE OPEN ACCESS

Innovative Aqueous Washing Agents for the Efficient Removal of Abamectin From Tomato (*Solanum lycopersicum* L.) Surface

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Received: 12 November 2025 | **Revised:** 16 March 2026 | **Accepted:** 27 March 2026

Keywords: abamectin | choline-based ionic liquids | pesticide removal | surfactants | tomato | wash

ABSTRACT

Pesticides are among the main sources of food contamination and pose severe risks to human health, making their removal from vegetable surfaces essential. This study evaluated different classes of surfactants and choline-based ionic liquids as alternative washing agents, being compared with traditional agents such as water, salts, and organic acids, for removing abamectin from tomato (*Solanum lycopersicum* L.) surfaces. Organic tomatoes were intentionally contaminated by spraying abamectin until reaching concentrations from 26 to 33 mg. L^{-1}. Various washing agents, including anionic, cationic, and non-anionic surfactants, as well as choline chloride and choline bitartrate, were employed using processing times ranging from 5 to 30 min. Ionic liquids, salts, and organic acids showed negligible removal capacity, whereas surfactants achieved removal efficiency between 30% and 100%, confirming that micellar solubilization is the main mechanism for abamectin detachment from the tomato surface. Among the evaluated surfactants, the shorter the alkyl chain, the higher the efficiency; furthermore, longer-chain non-ionic surfactants performed better. Sodium dodecyl sulfate (SDS) exhibited the best performance, achieving 100% abamectin removal at 0.025 M within 10 min. The removal efficiency was influenced by micelle shape and size at concentrations above the critical micellar concentration (CMC). Moreover, the SDS solution maintained full removal capacity for up to six reuse cycles without loss of efficiency. Fourier-transform infrared spectroscopy (FTIR) spectra of tomato surfaces before and after treatment revealed no chemical alterations, confirming that the washing process preserved the integrity of the fruit surface. These results demonstrate a sustainable, efficient approach for pesticide removal from fresh fruits.

1 | Introduction

Despite all the damage caused to the environment and human health, population growth demanded large-scale food production, putting pressure on the agricultural sector to use pesticides (Carrasco et al. 2021; Carvalho 2017). Pesticides are agrochemical compounds commonly used to prevent, destroy, repel, or inhibit pests (harmful insects and/or weeds) and diseases that affect agriculture (Venkatachalapathy et al. 2020; Rasolonjatovo et al. 2017).

Abbreviations: [Ch][Bit], choline bitartrate; [Ch][Cl], choline chloride; CMC, critical micellar concentration; CPB, 1-hexadecylpyridinium bromide; CTAB, hexadecyltrimethylammonium bromide; DSS, sodium dioctyl sulfosuccinate salt; FTIR, Fourier transform infrared spectroscopy; HPLC-DAD, high-performance liquid chromatography method coupled to a diode array detector; ILs, ionic liquids; NaCl, sodium chloride; $NaCl_4$, sodium perchlorate; SDBS, sodium dodecyl benzenesulfonate; SDS, sodium dodecyl sulfate; TTAB, tetradecyltrimethylammonium bromide.

Pesticides comprise a wide range of organic and inorganic chemical compounds, which are mainly classified into organochlorines, organophosphates, carbamates, pyrethroids, and neonicotinoids. They can also be classified according to their target organisms: insecticides, herbicides, fungicides, rodenticides, molluscicides, nematicides, and plant growth regulators (Garud et al. 2024). According to Bai and Ogbourne (Bai and Ogbourne 2016), among the pesticides currently in use are the avermectins, a class of macrocyclic lactones that exhibit nematocidal, acaricidal, and insecticidal activities. This group of pesticides comprises a family of compounds including moxidectin, milbemycin oxime, doramectin, selamectin, eprinomectin, as well as the more widely known abamectin and ivermectin. The focus of this study is abamectin, which is structurally composed of approximately 80% avermectin B_{1a} ($C_{48}H_{72}O_{14}$; 22,23-dihydroavermectin B_{1a}) and 20% avermectin B_{1b} ($C_{47}H_{70}O_{14}$; 22,23-dihydroavermectin B_{1b}).

Although pesticides have undeniably benefited large-scale agriculture, their high toxicity, combined with their extensive and uncontrolled use, make these compounds among the most serious problems generated by anthropogenic processes (Lewis and Maslin 2015). The harmful effect on human health varies from the acute to the chronic level of diseases associated with its use (Fenik et al. 2011), such as Cancer (Lerro et al. 2015), Asthma (Cherry et al. 2018), Diabetes (Evangelou et al. 2016), Parkinson's Disease (Baltazar et al. 2014), Leukemia (Malagoli et al. 2016), among others. Human contamination by pesticides can occur through the respiratory, ocular, skin, and oral routes (Damalas and Eleftherohorinos 2011).

Foods are considered the main source of human exposure to pesticides (Boobis et al. 2008). According to the Brazilian Food Pesticide Residue Analysis Program (PARA-Programa De Análise De Resíduos De Agrotóxicos Em Alimentos 2019), approximately 23% of all foods produced in Brazil have pesticide amounts above the permissible limit recommended by Brazilian legislation, of which bell peppers (82%), guava (42%), carrots (39%), and tomatoes (35%) are the main contaminated foods.

Tomato is one of the most consumed worldwide (Matos et al. 2012), with a world production of approximately 180 million tons in 2019. Asia contributed 62% and the American continent contributed 13.2%. The main tomato producer was China (34.7%), followed by India (10.5%), Turkey (7.1%), the USA (6.0%), and Egypt (3.7%) (FAOSTAT-Food and Agriculture Organization of the United Nations, Crops Statistics 2022). Brazil occupies the 10th position in the world (4.1 million tons or 2% of world production) (IBGE-Instituto Brasileiro de Geografia e Estatistica 2022), of which 65% of production is destined for "in nature" consumption, and 35% for processing by industry (Dossa and Fuchs 2017). The antiparasitic abamectin belonging to the class of avermectins is the pesticide commonly used in tomato crops. This pesticide is composed of at least 80% avermectin B_{1a} and not more than 20% avermectin B_{1b} (Fisher and Mrozik 1992), and is often sprayed on tomato crops during their life cycle, leading to the accumulation of these compounds at high levels on their surfaces (Kumari et al. 2007), due to their limited penetration into the surface cuticles of the food (Toker and Bayındırlı 2003). Therefore, it is necessary to establish operational procedures to remove these contaminants, since these foods are often eaten raw (Bajwa and Sandhu 2014; Bonnechere et al. 2012).

Traditional methods for removing pesticides from food products consist of washing with water and an aqueous solution of acids, bases, and oxidizing agents. Several researchers have studied the effectiveness of these washing solutions in removing pesticides in different foods (Acoglu and Omeroglu 2021; Kelageri et al. 2017; Wang et al. 2013; Liang et al. 2012; Satpathy et al. 2012; Zohair 2001; Abou-Arab 1999). However, the rinse with tap water and the aqueous traditional solutions only partially remove pesticides (Rasolonjatovo et al. 2017; Garud et al. 2024; Bai and Ogbourne 2016; Lewis and Maslin 2015; Fenik et al. 2011; Lerro et al. 2015; Cherry et al. 2018; Evangelou et al. 2016; Baltazar et al. 2014; Malagoli et al. 2016; Damalas and Eleftherohorinos 2011; Boobis et al. 2008; PARA-Programa De Análise De Resíduos De Agrotóxicos Em Alimentos 2019; Matos et al. 2012; FAOSTAT-Food and Agriculture Organization of the United Nations, Crops Statistics 2022; IBGE-Instituto Brasileiro de Geografia e Estatistica 2022; Dossa and Fuchs 2017; Fisher and Mrozik 1992; Kumari et al. 2007; Toker and Bayındırlı 2003; Bajwa and Sandhu 2014; Bonnechere et al. 2012; Acoglu and Omeroglu 2021; Kelageri et al. 2017; Wang et al. 2013; Liang et al. 2012; Satpathy et al. 2012; Zohair 2001; Abou-Arab 1999; Rodrigues et al. 2017). Therefore, the search for alternative washing solutions for pesticide removal such as surfactants and low-toxicity ionic liquids (ILs) is important for obtaining pesticide-free foods.

Surfactants are organic compounds with interesting characteristics, such as their amphiphilic nature, which is promoted by the presence of a hydrophobic tail and a hydrophilic head, capable of promoting the formation of micelles in an aqueous solution (Baptista et al. 2017; Rangel-Yagui et al. 2004; Liu et al. 1998). They are classified into anionic, non-ionic, cationic, and amphoteric, according to the electric charge present in the hydrophilic part of the molecule (Myers 2005). The difference between anionic and cationic ones is that the latter have a positive charge on their polar part, while anionics have a negative charge. Non-ionic compounds have no electrical charge, while amphoteric compounds have both negative and positive charges (Dave and Joshi 2017; Daltin 2011). Regarding toxicity, the anionic surfactants such as sodium dodecyl benzenesulfonate (SDBS), sodium dioctyl sulfosuccinate salt (DSS), and sodium dodecyl sulfate (SDS), used in this work, have moderated toxicity, while the cationic ones such as tetradecyltrimethylammonium bromide (TTAB), hexadecyltrimethylammonium bromide (CTAB), and 1-hexadecyl pyridinium bromide (CPB) have low toxicity to mammalian cells and aquatic organisms (Santos et al. 2016). They are compounds widely used in our daily lives, being present in the most diverse industries, food (Santos et al. 2016), health (Freddi et al. 2003), agrochemical (Sachdev and Cameotra 2013), among others.

ILs are organic salts with a melting point below those of conventional inorganic salts, which are formed by several combinations of anions and cations and, for this reason, called designer solvents (Aguilera-Herrador et al. 2010; Freire et al. 2007). Due to several beneficial properties of ILs, if properly designed, they are considered green and ecologically friendly (Bhat et al. 2022; Raj et al. 2016). An important precursor for synthesizing "greener" ILs (Gouveia et al. 2014; Zeisel and Costa 2009a) is Choline, which is naturally found in living beings. Several studies on the synthesis and characterization of choline-based ILs are available in literature, whereas most of these studies describe them as biodegradable and presenting negligible toxicity (Lopes et al. 2013; Petkovic et al. 2010).

The objective of the present work was to use different classes of surfactants (anionic, cationic, and non-ionic) and choline-based ionic liquids as alternative washing agents to the conventional salts and organic acids used in the removal of abamectin present in the surface of tomatoes (vegetable model). The best washing operation time, type, concentration of washing agent, and solution saturation were determined.

2 | Materials and Methods

2.1 | Materials

The analytical standard for abamectin was purchased from Sigma Co., St. Louis, MO, USA. Commercial abamectin (Abamex) was purchased from *Nufarm Indústria Química e Farmacêutica S/A* (Ceará, Brazil). Conventional salts, sodium chloride (NaCl > 99.9 wt% pure), and sodium perchlorate ($NaClO_4$ > 99 wt% pure) were obtained from Labkem (Barcelona, Spain). The organic acids, such as gallic acid (> 97.5 wt%) and ascorbic acid (> 99.7 wt%), were purchased from Sigma-Aldrich (Darmstadt, Germany). Choline-based ionic liquids, choline chloride [Ch]Cl (99 wt%), and choline bitartrate [Ch][Bit] (97 wt%) were obtained from Acros Organics (Geel, Belgium). The non-ionic surfactants such as Triton X-100, Tween 80, Tergitol 15-S-9, and Genapol X-080 were purchased from Sigma-Aldrich, and Tween 20 was purchased from Fagron (France). The cationic surfactants used were tetradecyltrimethylammonium bromide (TTAB, purity = 99%), acquired by Acros Organics (Geel, Belgium), and hexadecyltrimethylammonium bromide (CTAB, purity = 99%) and 1-hexadecyl pyridinium bromide (CPB, purity = 99%), purchased from Sigma-Aldrich (Darmstadt, Germany). The anionic surfactants tested were sodium dodecyl benzenesulfonate (SDBS, technical grade), and sodium dioctyl sulfosuccinate (DSS, purity 98%), both acquired from Sigma-Aldrich (France), and (SDS, purity 85%) purchased from AppliChem GmbH ITW reagents (Germany). Acetonitrile suitable for HPLC (gradient grade ≥ 99.9 wt%), and orthophosphoric acid (≥ 85 wt%) were purchased from Sigma-Aldrich (Darmstadt, Germany). Figure 1 depicts the structure of the washing agents and the studied pesticide (abamectin).

2.2 | Tomato Surface Contamination

Samples of organically grown tomatoes from Hortipor, a company specializing in organic farming products, were purchased at the local market (Aveiro, Portugal). Tomatoes were always acquired on the day of the experiment and transported to the laboratory. They were selected based on uniform size and maturation stage, then washed with water and dried with paper towels to remove surface dirt. Each tomato was sprayed 3 times with 2 mL of the aqueous solution of commercial Abamex (preparation 20 times more concentrated than recommended by the manufacturer), with an interval of 2 h, and dried under natural ventilation for 2 h to assess pesticide adherence. The

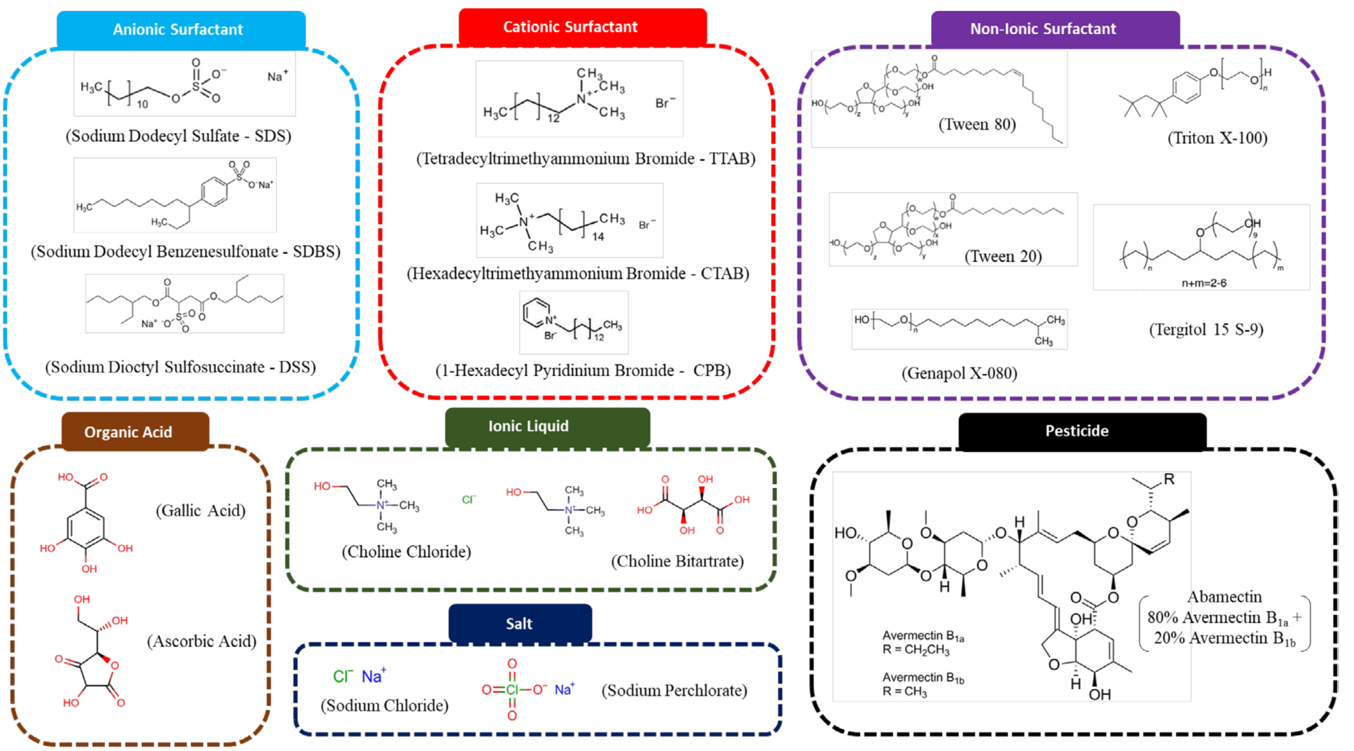

FIGURE 1 | Chemical structure of the washing agents (surfactants: Anionic, cationic, and non-ionic; organic acid; based-ionic liquid; and salts) and pesticide (abamectin).

concentration of commercial pesticide was measured in HPLC-DAD before its use in the experiment. The time of 4 h for application, drying, and washing of the pesticide during the process was determined from a previously carried out study on the stability of the commercial pesticide in water, as reported in the Supporting Information (Figure S1).

2.3 | Tomato Washing

The previously sprayed tomatoes were washed with different chemical compounds (washing agents). For each wash, two contaminated tomatoes were immersed separately for 30 min in 200 mL (distilled water or a different aqueous solution of washing agents at 0.025 M). In percentage the values are NaCl (0.15 wt%), $NaClO_4$ (0.35 wt%), gallic acid (0.42 wt%), ascorbic acid (0.44 wt%), [Ch]Cl (0.35 wt%), [Ch][Bit] (0.63 wt%), SDS (0.72 wt%), SDBS (0.87 wt%), DSS (1.10 wt%), TTAB (0.84 wt%), CTAB (0.90 wt%), CPB (0.99 wt%), Tween 80 (3.18 wt%), Tween 20 (2.98 wt%), Triton X-100 (1.54 wt%), Tergitol 15S-9 (1.46 wt%) and Genapol X-080 (1.37 wt%). Afterward, aliquots were taken at 5, 10, 15, and 30 min. The effect of the best washing agent concentration (SDS, 0.082 M—0.04 M) was studied at the optimal process time (10 min).

After washing, the samples were carefully filtered through a 0.20 μm syringe filter to remove any solids from the liquid phase, and the filtrates were subsequently quantified by HPLC-DAD (Shimadzu, model PROMINENCE). HPLC-DAD analyses were performed on a C18 reversed-phase analytical column (250 × 4.60 mm, Kinetex 5 μm C18 100 Å, Phenomenex). The mobile phase consisted of 60% (v/v) acetonitrile and 40% (v/v) ultra-pure water with 0.3% (v/v) orthophosphoric acid. Separation was performed in isocratic mode at a flow rate of 0.8 mL·min^{-1} with an injection volume of 20 μL. The column oven and autosampler were operated at 35°C. The wavelength was set at 245 nm, and each sample was analyzed in triplicate. The calibration line was obtained using a pure analytical standard of abamectin dissolved in acetonitrile; the data are reported in the Supporting Information (Figure S2). Under these conditions, abamectin has a retention time of 25.2 min. It is worth noting that all solutions before washing (in the absence of pesticides) were injected to obtain the blank and to discard the influence of the chemical compound.

The removal efficiency (%) of the pesticide abamectin was calculated by Equation (1):

$$\text{Removal efficiency (\%)} = \frac{\text{mass removed}_{\text{pesticide}}}{\text{mass impregnated}_{\text{pesticide}}} \times 100 \quad (1)$$

where the mass removed is the mass quantified in the washing solution, and the impregnated mass is the mass quantified in the solution used to contaminate the tomato surface.

2.4 | Saturation of the Aqueous Solution of SDS

The saturation of the washing solution under the best operating conditions (washing agent-SDS, time-10 min, and concentration-0.025 M) was determined by successive washes of 10 tomatoes (one in each cycle) with the same solution. For each washed tomato, an aliquot of 1 mL of the washing solution was collected, and the abamectin concentration was determined by the aforementioned method.

2.5 | Tomato Skin Evaluation by FTIR

Fourier-transform infrared spectroscopy (FTIR) analysis of oven-dried tomato skin was performed to verify the impregnation and removal of pesticides from the tomato surface and to examine the tomato skin structure. Initially, tomatoes at each stage were peeled with a knife, separating the skin from the pulp. The pulps were discarded, and the skins were carefully transferred to separate Petri dishes and then stored in an oven at 25°C for 24 h. Afterward, the skins were analyzed by Fourier transform infrared spectroscopy with attenuated total reflectance (FTIR) to evaluate changes in the groups present in the tomato skin. The spectrum of each sample was acquired on a PerkinElmer Spectrum BX FTIR system equipped with a diamond crystal and a single horizontal Golden Gate ATR cell. Analysis of "in nature" pesticide-contaminated skin after washing with SDS and water was performed at room temperature (25°C ± 2°C) with controlled relative humidity (75–80 wt%). All data were recorded over 4000–400 cm^{-1} with a resolution of 4 cm^{-1}, accumulating 32 scans with an interval of 1 cm^{-1}. For all acquired spectra, the background air spectrum was subtracted, and the results were recorded as transmittance values.

3 | Results and Discussion

3.1 | Abamectin Removal From Tomato's Surface

A screening of different non-conventional washing agents, such as choline-based ionic liquids and surfactants (anionic, cationic, and non-ionic), was performed to remove abamectin from the tomato surface. The results were compared with those obtained with traditional washing agents (salts and organic acids) at the same concentration (0.025 M) and 25°C for 10 min. The respective results are shown in Figure 2. All detailed removal efficiency results are provided in the Supporting Information (Table S1).

We first evaluated aqueous solutions of salts and organic acids commonly used in food processing and postharvest washing; however, these solutions showed no significant efficiency in removing abamectin from the surface. Subsequently, we investigated choline-based ionic liquids, given their potential for regulatory acceptance by the U.S. Food and Drug Administration (FDA) for food-related applications. Nevertheless, these compounds also failed to promote effective abamectin removal from the tomato surface (Zeisel and Costa 2009b).

Because abamectin is neutrally charged, ionic strength does not affect pesticide removal; therefore, we focus on the surfactant's hydrophobic/hydrophilic characteristics. Salts (NaCl and $NaClO_4$), organic acids (gallic and ascorbic acid), and ionic liquids ([Ch][Cl] and [Ch][BIT]) did not remove abamectin, possibly due to its hydrophilic characteristics ($-7.84 \leq \text{Log } p \leq -0.77$), which

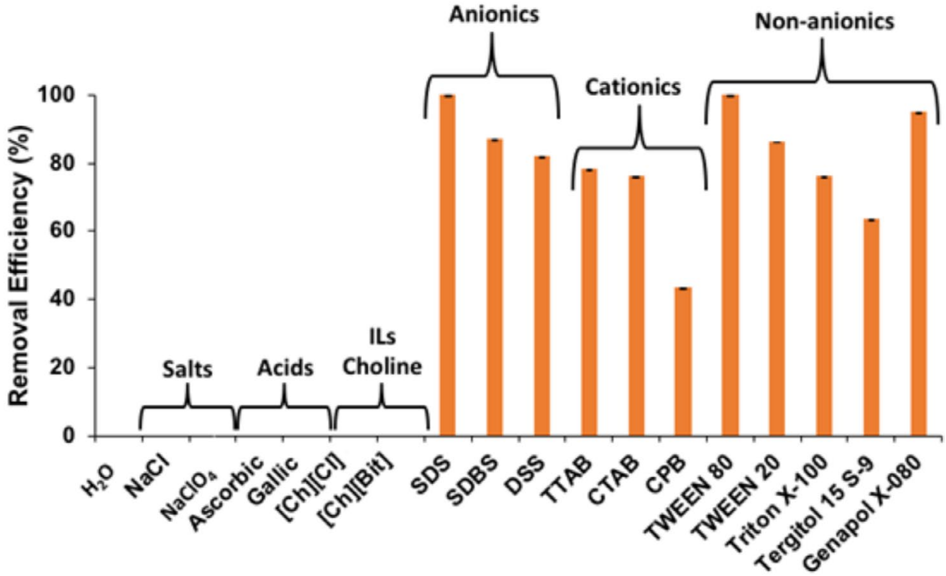

FIGURE 2 | Effect of different washing agents (0.025 M) used to remove the pesticide abamectin from the tomato surface at 25°C for 10 min.

are incompatible with abamectin (Log $p = 5.85$). Acoglu and Omeroglu (2021) investigated the effectiveness of different non-toxic washing agents (tap water and solutions of sodium carbonate, sodium chloride, acetic acid, apple cider, and vinegar), reporting only 2% abamectin removal. These results in removing abamectin from the orange surface are in agreement with ours, supporting the low efficiency of conventional salts and organic acids.

We then shifted to using readily available commercial surfactants with varying toxicological profiles. We began with low-toxicity surfactants commonly regarded as GRAS (Generally Recognized as Safe), namely Tween 80 and Tween 20, which are also reported to exhibit low cytotoxicity (Lindenberg et al. 2019). This group was complemented by SDS, which has specific applications in food-related contexts, and by sodium dodecyl benzenesulfonate (SDBS), which is characterized by moderate cytotoxicity. To broaden the screening, we further evaluated surfactants with moderate cytotoxicity, such as Tergitol 15-S-9 and Genapol X-080, as well as more cytotoxic cationic surfactants, including hexadecyltrimethylammonium bromide (CTAB), hexadecylpyridinium bromide (CPB), and tetradecyltrimethylammonium bromide (TTAB) (Ruissen et al. 1998).

Surfactants have hydrophobic properties ($1.80 \leq \text{Log } p \leq 6.41$) and were effective in abamectin removal, achieving 50%–100%. For ionic surfactants, hydrophobicity is less effective for pesticide removal; thus, SDS (Log $p = 2.04$) for the anionic (100%) and TTAB (Log $p = 1.80$) for the cationic (78.19%) showed the best results. It is known that the smaller the hydrophobic chain, the greater the diffusion rate and, consequently, the better the wetting capacity of the surfactant (Porter 1994). Additionally, it was observed that the anionic characteristic of the surfactants is more favorable in removing abamectin from the surface of tomatoes, which is due to low detergent power and consequently less efficient in the rupture and solubilization of the hydrophobic compounds adhered to the tomato surface (Li et al. 2021). On the other hand, non-ionic surfactants with longer carbon chains showed the best removal of abamectin (52.39%–100%). For this class of surfactants, pesticide removal values were higher than those of cationic surfactants and like those of anionic surfactants. According to Fabbri et al. (2009), anionic and non-ionic surfactants adsorb poorly to surfaces, favoring the formation of micelles in the washing solution and, consequently, the removal of the pesticide. Cationic surfactants are adsorbed on the surface by cation exchange, followed by the formation of a bilayer and droplets on the surface. Moreover, the difference in abamectin removal between surfactants is due to their characteristics. For the non-ionic surfactants, the cleaning action is the most important, for the cationic ones, the wetting action, while for the anionic ones, it is the combination of the cleaning and detergency action (York 2005).

The most effective agents to remove abamectin (surfactants) were used to investigate the effect of washing time, whose results are shown in Figure 3. All detailed removal efficiency results are provided in the Supporting Information (Table S1). Overall, the abamectin removal from the tomato surface was high (>60%) within the first 5 min of the process, regardless of the used surfactant as a washing agent, as observed by Li et al. (2021). After, a maximum removal or extraction threshold was observed depending on each surfactant used. In some cases, prolonged exposure can lead to possible reabsorption of abamectin on the surface of the tomato and, consequently, a reduction in abamectin removal. Mohammd and Jaber (2022) reported a maximum absorption of abamectin using the non-ionic surfactant sorbitan monooleate (Span 80) in the presence of Fe_3O_4 magnetic nanoparticles, which occurred within 10 min, followed by desorption under different evaluated conditions, including surfactant concentration, magnetic nanoparticle concentration, and pH.

Only the surfactants SDS (anionic) and Tween 80 (non-ionic) were able to remove 100% of abamectin. It should be noted that for the last one, long times promote severe resorption, while for the first one, this phenomenon was not observed. In this case, the results suggest that the surfactant effect on the washing agent is essential for it to remove the pesticide. The presence of surfactant molecules on the surface reduces the cohesive force between water molecules and the pesticide adhered to the tomato skin, thereby reducing surface tension and allowing its removal

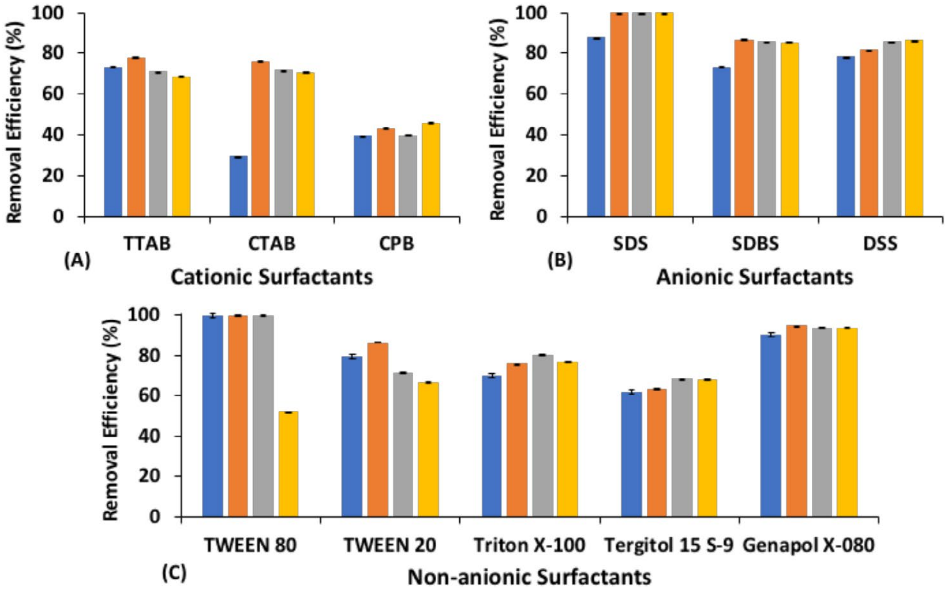

FIGURE 3 | Different classes of surfactants as surface washing agents for tomatoes to remove the pesticide abamectin. (A) cationic surfactants; (B) anionic surfactants; (C) non-ionic surfactants; Blue bar—5 min; Orange bar—10 min; Gray bar—15 min; and, Yellow bar—30 min.

(Alves 2015). It is known that these compounds can promote/help cell disruption and/or can help in the solubilization of most hydrophobic compounds (Vieira et al. 2018), not being different from abamectin, which has low water solubility and is a highly hydrophobic compound.

These alternative washing agents showed significant pesticide removal, exceeding the values reported by Abou-Arab (1999), who reported that rinsing tomatoes with a NaCl (2%–10%) solution reduced organophosphate pesticide residues by 27%–91.4%, while acetic acid reduced pesticide concentration by 20.4%–93.7%. Additionally, Wang et al. (2013) used two common kitchen detergents to analyze the potential for removing chlorothalonil and chlorpyrifos from cherry tomatoes, achieving the best removal values of 80% and 42%, respectively, at 20 min of wash time.

Fortunately, the most effective surfactants identified were those with low to moderate toxicity, namely Tween 80 and SDS, respectively. Among them, SDS was selected due to its superior time-dependent removal performance. It is well established that increasing surfactant concentration may lead to higher cytotoxicity (Arechabala et al. 1999). However, for SDS, concentrations above the critical micelle concentration (CMC) promote micelle formation in the bulk solution, thereby enhancing solubilization and facilitating its removal from surfaces during washing (Godoy et al. 2025).

3.2 | Effect of SDS Concentration on Abamectin Removal

To enhance the process, the effect of SDS concentration on abamectin removal was investigated. Figure 4 depicts the data obtained, starting from the critical micellar concentration (CMC of SDS) at 0.008 M until 0.04 M at different washing times. All detailed removal efficiency results are provided in the Supporting Information (Table S2).

The removal of abamectin reached 100% at 0.025 M of SDS. At SDS concentrations above 0.025 M, the capacity to remove the washing agent declined by approximately 50%. When surfactant molecules are dissolved in water at concentrations above the CMC, they form aggregates known as micelles. As a result, the hydrophobic tails migrate inward to minimize contact with water, while the hydrophilic heads remain on the external surface to maximize contact with water (Clarke 1981). Therefore, the amount, shape, and size of micelles formed at concentrations lower than 0.025 M probably do not have enough power to break the existing surface tension. The shape and size of the micelle, as well as the properties of the associated micellar solution, can be adjusted by varying solution conditions, such as surfactant concentration and temperature (Liu et al. 1998; Chevalier and Zemb 1990). Normally, the micelle structure changes with increasing surfactant concentration. However, they are generally spherical; some micelles at concentrations well above the CMC and under appropriate conditions may adopt other shapes (Trados 1994), which could be happening in this study. At concentrations above 0.025 M, the micelle structure is likely to change, drastically reducing its performance as a washing agent. The results suggest that a minimum SDS concentration is required to achieve complete removal of pesticide, but exceeding this minimum accentuates the adverse effect.

The abamectin removal efficiencies obtained with SDS at concentrations below 0.025 M are comparable to those reported by Kelageri et al. (2017), who investigated the removal of pesticides such as dimethoate, λ-cyhalothrin, forchlorfenuron, flubendiamide, and profenofos from tomato surfaces using conventional washing agents. Their results showed removal efficiencies ranging from 52% to 71% with acetic acid solutions, 39%–58% with saline and soda solutions, and 17%–39% with tap water. Under optimal conditions, the removal efficiency of abamectin using SDS aligns with the findings by Venkatachalapathy et al. (2020), who achieved high reductions in organophosphate pesticide residues on tomatoes using natural plant extracts. In their study, maximum removal was observed for dichlorvos (87%), followed by dimethoate (84%), malathion (83%), and chlorpyrifos (64%) after 15 min of washing with saponins extracted from *Albizia amara* and *Acacia concinna*.

Continuing our efforts to improve abamectin removal from the tomato surface, we investigated the possibility of reusing the washing agent solution across multiple cycles.

3.3 | Saturation of the Aqueous Solution of SDS

As previously discussed, several works in the literature reported on the removal of pesticides from food products using conventional methods, such as washing with water or aqueous solutions of acids, bases, and oxidizing agents. However, in the present study, these traditional washing agents proved ineffective in removing the target pesticide, abamectin. Consequently, alternative agents were explored, and surfactants emerged as highly efficient for this application. Despite their superior performance, surfactants generally cost more than conventional washing agents.

Despite its higher cost compared to traditional washing agents, the reusability of the SDS solution was evaluated by examining its saturation behavior over multiple washing cycles. Figure 5 depicts the pesticide removal efficiency across 10 consecutive cycles, corresponding to washing 10 tomatoes using the same solution. The data demonstrate that the SDS solution remains highly effective through the first six cycles, achieving complete abamectin removal (100%). Although efficiency declines from the seventh cycle onward, the solution still delivers satisfactory performance up to the tenth cycle. Comprehensive data, including the initial pesticide mass (impregnated), final solution mass, mass difference for each washing cycle, and corresponding removal efficiencies, are provided in the Supporting Information (Table S3).

The results indicate that the SDS solution can be efficiently reused for pesticide removal, exhibiting only a 16% reduction in performance after ten consecutive uses. While complete (100%) removal was maintained through the sixth washing cycle, subsequent cycles showed a gradual decline in efficiency—98.38%, 89.07%,

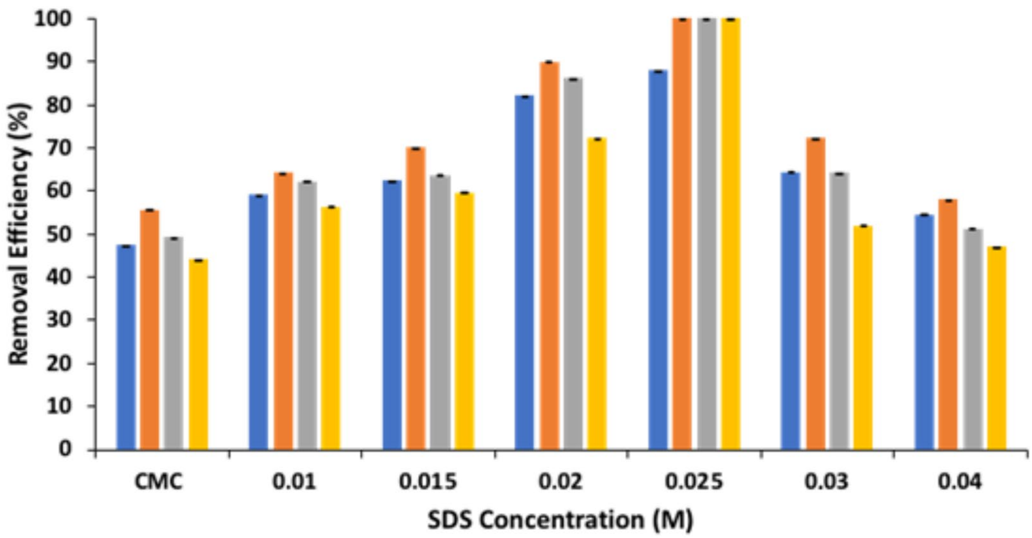

FIGURE 4 | Study of the effect of SDS concentration on the removal of the pesticide abamectin from the tomato surface. Blue bar—5 min; Orange bar—10 min; Gray bar—15 min, and Yellow bar—30 min.

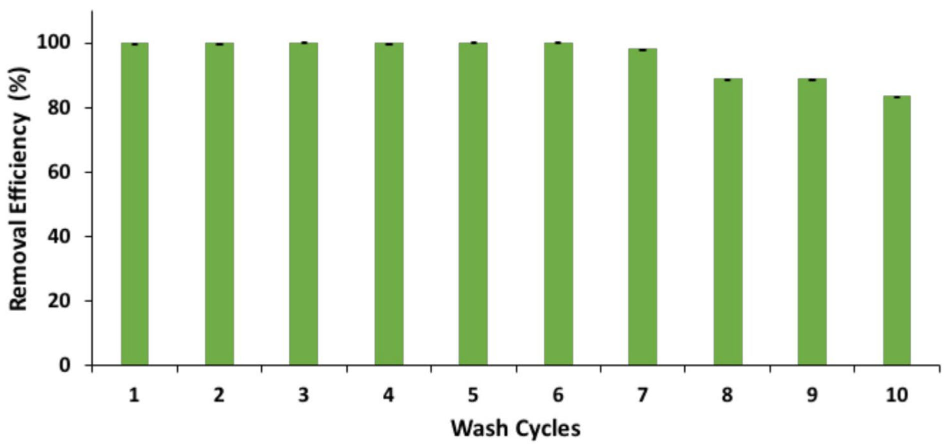

FIGURE 5 | Reuse of the SDS solution at 0.025 M in the wash time of 10 min for different cycles.

88.52%, and 83.18% in cycles 7–10, respectively. This decrease is likely due to the progressive saturation and contamination of micelles, which are responsible for solubilizing the hydrophobic pesticide abamectin during the washing process. From the seventh cycle onward, the reduced availability of active micelles may compromise removal efficiency. These findings support the potential of SDS as a highly effective and reusable alternative washing agent for pesticide removal. However, it was also important to assess whether repeated surfactant use could compromise the tomato skin's structural integrity or leave pesticide residues. To address this concern, FTIR spectroscopy was employed to evaluate tomato skin at different stages of the washing process, enabling analysis of both pesticide presence and potential structural modifications.

3.4 | Tomato Skin Evaluation by FTIR

Mechanistically, the hydrophobic alkyl chain of SDS can interact with the lipid-rich waxy cuticle of the tomato surface. At the same time, the sulfate headgroup remains oriented toward the aqueous phase, forming a relatively stable adsorbed interfacial layer (Hess and Foy 2000). In this context, the effect of the treatment on the tomato surface was further investigated through FTIR analysis to assess possible chemical modifications.

FTIR spectroscopy is widely used to investigate molecular interactions and identify structural features and potential interactions in materials (Alomar et al. 2016). This technique enables the identification of functional groups present in a sample by comparing its spectrum with established reference spectra. In this study, FTIR spectra were acquired for tomato skin at various stages, as well as commercial abamectin and the SDS surfactant. Figure 6 depicts the normalized transmittance spectra of these samples, highlighting the characteristic functional groups identified. Through this analysis, it was possible to assess the molecular structure of tomato skin before washing, confirm the abamectin impregnation on the tomato surface, and demonstrate the successful removal of the pesticide following SDS treatment. Notably, the spectra also confirmed that no structural alterations occurred in the tomato skin after the washing process, further validating the efficacy and safety of SDS as a washing agent.

By analyzing the FTIR spectrum of tomato skin in the absence of abamectin, a prominent absorption band is observed around 3400 cm^{-1} corresponding to O—H stretching vibrations characteristic of hydroxyl groups in cellulose (Sabiha-Hanim and Aziatul-Akma 2016). In the fingerprint region, between 1700 and 600 cm^{-1}, absorption bands typical of hemicellulose, cellulose, and lignin are evident. Notably, the peak near 1700 cm^{-1} is attributed to C═O stretching vibrations from carboxylic acids and esters (Mateus et al. 2017). Additionally, in the 1100–1000 cm^{-1} region, bands associated with the elongation of C—O—C bonds in cyclic ethers and C—O stretching from primary and secondary alcohols are verified. In contrast, the FTIR spectrum of tomato skin exposed to abamectin reveals additional characteristic peaks corresponding to the pesticide. These include the elongation of the C—H band at 2918 and 2952 cm^{-1}, a prominent C═O stretching band at 1730 cm^{-1} attributed to the macrolide ring, and a C—O—C stretching band at 1378 cm^{-1}. These bands are also present in the FTIR spectrum of commercial abamectin, thereby confirming the presence and surface impregnation of abamectin on the tomato skin.

The FTIR spectrum of tomato skin following washing with SDS closely resembles that of the untreated skin (i.e., without abamectin), indicating effective pesticide removal during the washing process. This spectrum similarity confirms both the

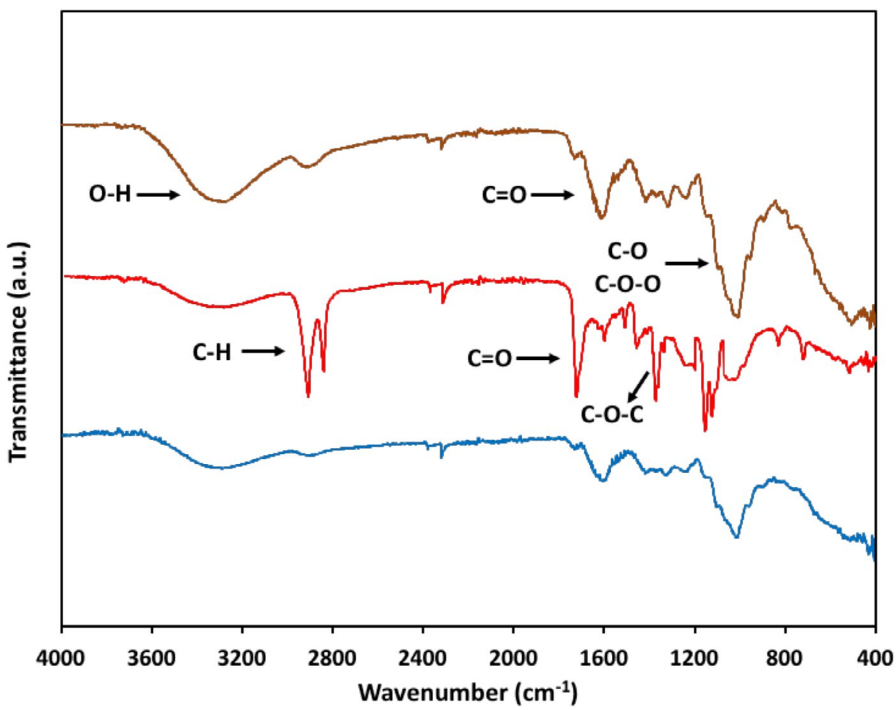

FIGURE 6 | FTIR spectra for tomato skin in the absence of pesticide (brown), for tomato skin in the presence of pesticide (red), and tomato skin after the SDS surfactant washing operation (blue).

successful extraction of abamectin and the preservation of the tomato skin's structural integrity, demonstrating that SDS does not induce significant alterations to the native chemical structure of the tomato surface. Moreover, FTIR spectra of the individual components, including pure SDS, commercial abamectin, standard abamectin, and tomato skin washed only with water post-impregnation (which showed limited efficacy in pesticide removal), are provided in Figure S3 in the Supporting Information.

4 | Conclusions

To the best of our knowledge, this is the first work that reports the application of different classes of surfactants, choline-based ionic liquids, water, salts, and acids as washing agents for removing the pesticide abamectin from the tomato surface. The investigation revealed that the presence and type of surfactant strongly influence the removal efficiency in the washing solution. Surfactants demonstrated a positive effect, and studies of several surfactant classes enabled an in-depth understanding of the influence of carbon chain length on pesticide removal. For anionic and cationic surfactants, shorter carbon chains enhanced removal efficiency, whereas for non-ionic surfactants, longer chains were more effective. SDS and Tween 80 demonstrated significantly higher efficiency in removing abamectin than conventional washing agents, achieving 100% removal under the tested conditions, whereas traditional washing solutions were ineffective. Tween 80 exhibits low cytotoxicity and is widely regarded as a GRAS surfactant by the FDA for specific food applications. In contrast, SDS presents moderate cytotoxicity, and its use in food-related contexts is restricted to specific regulatory conditions. However, at concentrations above its CMC, which is the case of the present work, SDS forms micelles in solution, thereby reducing its tendency to remain adsorbed to surfaces. SDS was selected for further optimization due to its lower required dosage. The results showed that concentrations above the CMC improved performance, with 100% removal at 0.025 M. However, concentrations beyond this threshold led to a sharp decline in efficiency, dropping to approximately 50%. Under optimal conditions (0.025 M SDS for 10 min of washing), the solution effectively removed abamectin across six washing cycles, with only a minor 16% reduction in efficiency observed in subsequent uses. This behavior was supported by FTIR analyses, which showed no detectable chemical modification of the tomato surface after treatment. From an economic perspective, SDS is also more cost-effective, making it an attractive alternative when considering both removal efficiency and operational feasibility.

Author Contributions

Isabela N. Souza: conceptualization, methodology, writing – original draft, data curation, formal analysis. **Julia Cardoso Rocha:** formal analysis. **Cleide M. F. Soares:** validation. **Matheus M. Pereira:** formal analysis, writing – review. **Ranyere L. de Souza:** formal analysis. **Mara G. Freire:** writing – review and editing, funding acquisition, supervision. **Álvaro S. Lima:** conceptualization, resources, project administration, funding acquisition, writing – review and editing, supervision.

Acknowledgments

The Article Processing Charge for the publication of this research was funded by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) (ROR identifier: 00x0ma614).

Funding

This work was developed within the scope of the project CICECO–Aveiro Institute of Materials, UID/50011 & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC). The authors acknowledge Conselho Nacional de Desenvolvimento Científico e Tecnológico [CNPq] through the projects 302988/2019-0 and 428267/2018-1, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior [CAPES], and Fundação de Apoio à Pesquisa e à Inovação Tecnológica do Estado de Sergipe [FAPITEC/SE]. Matheus M. Pereira acknowledges the financial support of FCT, Portugal, within the projects DOI: 10.54499/UIDB/00102/2020 (Base funding) and DOI: 10.54499/UIDP/00102/2020 (Programmatic funding). Fundação para a Ciência e a Tecnologia (UIDB/50011/2020, UIDP/50011/2020, LA/P/0006/2020, 10.54499/UIDB/00102/2020, 10.54499/UIDP/00102/2020).

Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data that supports the findings of this study are available in the Supporting Information of this article.

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Supporting Information

Additional supporting information can be found online in the Supporting Information section. **Figure S1:** Stability of commercial abamectin in water. **Figure S2:** Calibration line of the analytical standard abamectin in HPLC. **Figure S3:** FTIR spectra: (—) pure SDS; (—) Standard Abamectin; (—) Commercial Abamectin and (—) tomato skin after washing with water only. **Table S1:** Detailed data on the removal efficiencies of all surfactants at different washing times. **Table S2:** Detailed data on the removal efficiencies for the study of SDS concentration at different washing times. **Table S3:** Detailed data on initial masses (impregnated), final masses (total mass of solution), mass difference (each wash cycle) and removal efficiencies for the different wash cycles.