

Post-detonation recovery of chemical warfare agent simulants using wet swabbing and bulk fragment extraction

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ABSTRACT

Reliable, targeted sampling and detection of chemical warfare agent (CWA) residues following explosive dissemination remains a critical challenge in forensic chemistry and chemical incident response. This study integrates controlled detonation experiments with quantitative residue and statistical analysis, demonstrating the importance of matrix-specific and complementary sampling approaches for accurate residue detection. Two physicochemically diverse CWA simulants, methyl salicylate and malathion, as analogues for sulfur mustard (HD) and VX, were applied to steel ball bearings using cotton-polyester fabric or cotton wool across three deposition methods to evaluate their influence on simulant retention following detonation. Residues were quantified by high-performance liquid chromatography (HPLC) to assess both retention and secondary transfer. Results show matrix-dependent residue behaviour, with fabric consistently exhibiting the highest retention of methyl salicylate (up to 6 mg/L), while non-porous materials such as ball bearings and plastic fragments generally retained minimal residues. Container fragments selectively retained malathion more effectively, consistent with differences in physicochemical properties. Secondary transfer was confirmed by the detection of residues on initially uncontaminated fragments. Statistical significance of retention and transfer trends was evaluated using binary logistic regression. Findings demonstrate that matrix characteristics, deposition method, and simulant physicochemistry strongly govern post-blast residue patterns of CWAs. Importantly, residual contamination on fragments remained sufficient to pose transdermal and/or inhalation hazards, given the extreme acute toxicity of VX, which exhibits an oral LD₅₀ of 0.04 mg/kg. Overall, the study provides novel, quantitative insight into post-detonation behaviour, informing forensic sampling strategies, hazard management, and chemical, biological, radiological, and nuclear (CBRN) incident response.

1. Introduction

Chemical, biological, radiological, and nuclear (CBRN) weapons remain a significant forensic and public safety concern due to their potential use in both conflict and terrorist incidents. Despite extensive international non-proliferation agreements and treaties, including the 1925 Geneva Protocol, the 1968 Treaty on Non-Proliferation of Nuclear Weapons (NPT), the 1975 Biological and Toxin Weapons Convention (BTWC), the 1997 Chemical Weapons Convention (CWC), and the 2021 Treaty on the Prohibition of Nuclear Weapons (TPNW), recent incidents involving chemical agents have highlighted the continued risk posed by their illicit use and the importance of effective forensic detection, attribution, and hazard assessment [1–12].

Improvised explosive devices (IEDs) represent a particularly

concerning dissemination mechanism, as they can simultaneously disperse toxic substances and generate complex fragmentation debris fields. Effective forensic recovery and analysis of chemical agent residues from post-blast environments are essential for incident reconstruction, attribution and risk management [13–18].

The rise of asymmetric warfare has been accompanied by increased use of IEDs, in which fragmentation represents a dominant damage mechanism, particularly in person-borne improvised explosive devices (PB-IEDs), where metallic fragments such as ball bearings, nuts, and bolts are deliberately incorporated to maximise lethality [19–21]. These fragments are subjected to extreme pressures and temperatures, resulting in high-velocity dispersal. Field studies employing blast-driven metallic fragments have demonstrated that even small charge sizes can produce serious injury zones extending up to 20–30 m [20–22].

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During explosive dispersal, chemical agents or simulants can deposit onto fragment surfaces through direct contamination, aerosol condensation, or secondary transfer processes. The extent of residue retention is dependent on fragment material composition, surface porosity, surface energy, and the physicochemical properties of the agent. Surface energy governs intermolecular interactions and adsorption strength, influencing residue persistence and recoverability [23–26]. Residues undergo adsorption onto fragment surfaces or absorption into porous materials, with surface interactions strongly influencing retention and analytical recovery [14,25,27]. Additionally, elevated temperatures generated during detonation promote thermal degradation, volatilisation, and bond cleavage of organophosphorus compounds or hydrolysis of simulants [28–31]. These physicochemical processes collectively influence residue persistence, spatial distribution, and recoverability in forensic post-blast environments.

Previous forensic studies predominantly focused on explosive residue characterisation from post-blast debris and environmental samples from a variety of evidential matrices [32–40]. Similarly, environmental and surface sampling methods for CWAs and simulants have been investigated across a range of matrices, including soil, vegetation, and building materials [26,33,41–52]. These studies have demonstrated that matrix composition, surface chemistry, and environmental conditions significantly affect residue persistence, transfer, and analytical recovery.

Locating, identifying, and securing CBRN materials and associated devices is essential to supporting hazard assessment and forensic investigations [53]. However, no published research has addressed the recovery and persistence of CWA residues specifically on blast-generated fragments. Explosive fragmentation introduces unique conditions that alter residue deposition patterns, reduce retention, or promote secondary transfer between materials. Fragment rapid transport and surface heterogeneity, combined with high-energy dispersal and variable deposition mechanisms, create complex evidential matrices which substantially differ from those encountered in non-blast contexts. Therefore, conclusions from standard surface studies cannot be applied directly to post-blast analysis without accounting for fundamentally different conditions. Consequently, empirical guidance on post-blast residue recovery, matrix-specific retention, and optimal forensic sampling strategies for chemically contaminated fragments remains limited.

Effective response to such incidents requires rapid hazard containment, casualty evacuation, and technical site exploitation, a complex process demanding interagency coordination and high technical expertise [53]. Understanding residue transfer and retention dynamics on blast fragments is critical for improving forensic recovery protocols, supporting attribution efforts, and enabling effective hazard assessment following chemical dispersal incidents. Systematic investigation of how deposition method, fragment material, and chemical properties influence residue persistence can provide essential insights into evidential recovery and interpretation.

This study aims to evaluate the effects of deposition method and agent chemistry on post-blast residue transfer and retention following controlled explosive dispersal to inform post-blast sampling and forensic recovery. Experiments employ controlled, laboratory-scale IED replicates with approved safety controls and operationally relevant matrices. Specifically, the study: (1) quantifies residue recovery across common evidential matrices (ball bearings, fabric, container, plastic, and wet cotton swabs); (2) compares retention and transfer patterns for two chemically distinct, low-toxicity simulants (methyl salicylate and malathion); and (3) derives practical implications for forensic sampling strategies, post-incident attribution, and rapid hazard assessment.

2. Materials and methods

2.1. Chemicals

Two CWA simulants were selected for this study to represent a blister and a nerve agent. Methyl salicylate ($\geq 99\%$, GC grade; Sigma Aldrich,

UK) was used to emulate sulfur mustard (HD), and malathion (analytical standard; Sigma Aldrich, UK) was used as a surrogate for VX [54]. Fig. 1 illustrates the chemical structures of the two simulants and their toxic counterparts. Both simulants are readily detectable using reverse-phase high-performance liquid chromatography (RP-HPLC), providing sufficient sensitivity and specificity for controlled experimental evaluation, despite limited overlap with the functional groups of their toxic counterparts. All reagents, including methanol ($\geq 99.8\%$, HPLC-grade, Fisher Scientific, UK), water (HPLC-grade, Fisher Scientific, UK), formic acid ($99 + \%$, Thermo Scientific, UK) and acetonitrile ($\geq 99.9\%$, HPLC-grade, Sigma Aldrich, UK), were used without further purification.

2.2. Experimental setup

All devices were detonated remotely inside the reinforced containment building at the explosives research and detonation area (ERDA) of the Defence Academy of the United Kingdom, Shrivenham, under licensed safety protocols. Personnel wore full protective equipment, and access was strictly controlled (Fig. 2). The containment building allows experiments involving explosively propelled fragmentation while maintaining safety; however, its sand-covered floor hinders sample recovery. Detonation experiments comprised two blank detonations to determine an appropriate charge for fragment propulsion and twelve independent detonations to quantify residue transfer across three deposition methods and two CWA simulants, mimicking a PB-IED event.

Each device was placed on a 66 cm-high blast-resistant block, with the ball bearing-covered surface oriented toward the target panels (Fig. 2). To capture penetrating fragments, a primary target panel (7 mm strawboard for early shots; substituted with 6 mm Medium Density Fibreboard (MDF) for later malathion trials due to procurement constraints) was positioned 1 m from the device. A secondary 13 mm panel was placed directly behind the primary panel to capture fragmentation [21,55,56].

Preliminary blank detonations were conducted to empirically determine a charge mass that produced sufficient fragment propulsion while remaining compatible with post-detonation sampling requirements. [58]. A 20 g PE-8 charge resulted in extensive propulsion of the fragmentation, evidenced by 41 penetrations of the strawboard target at 2 m. In contrast, a 10 g charge produced fewer penetrations (six impacts), indicating sufficient fragment propulsion for this study. The intermediate charge mass selected for subsequent experiments was

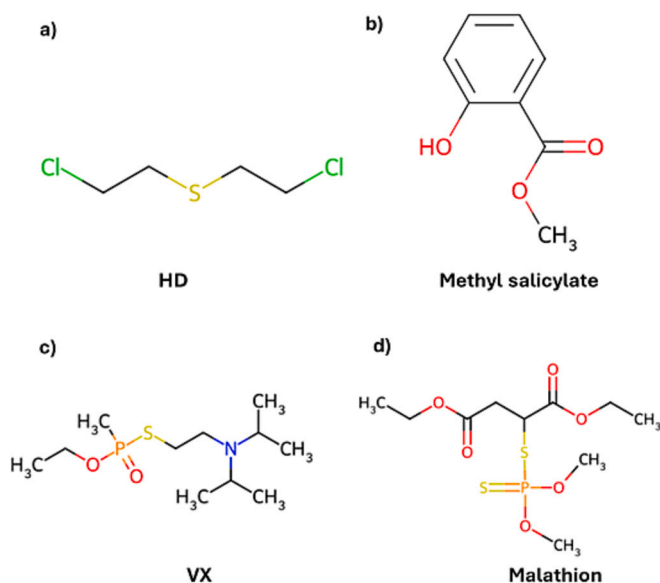


Fig. 1. Chemical structures of a) HD, c) VX and their simulant counterparts b) methyl salicylate and d) malathion.

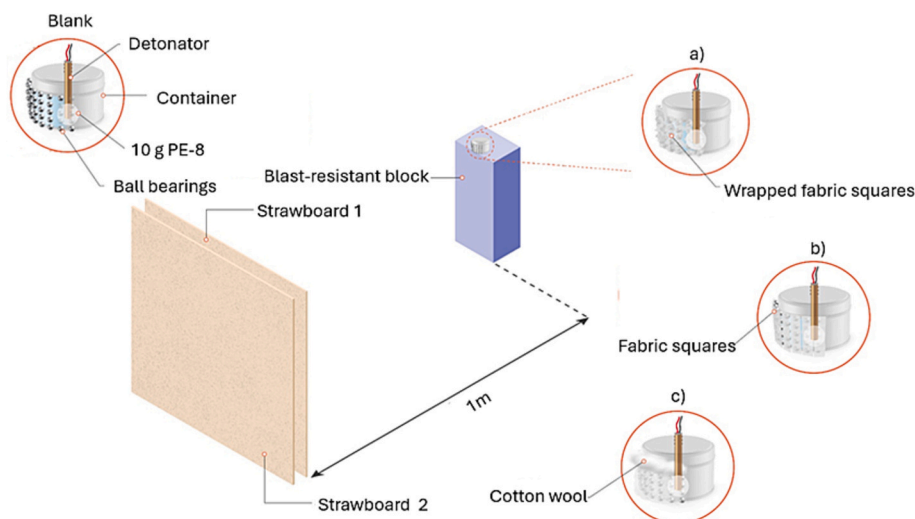


Fig. 2. Schematic of the experimental setup within the containment building at the Defence Academy, Shrivenham, UK.

therefore chosen to balance realistic fragment propulsion with safe operation and recoverable residue sampling. Tests 3–11 evaluated methyl salicylate contamination at a target distance of 1 m, optimised to ensure sufficient fragmentation capture [55,56].

These tests comprised all three deposition conditions (wrapped fabric, flat-wrapped fabric, and cotton wool strips) with three independent firings per condition ($n = 3$ per deposition method) (See Table 1). Tests 12–14 used the same device design and 10 g charge to evaluate malathion under Method A (wrapped-fabric; $n = 3$). Procedural controls, including uncontaminated blank fragments and solvent-only swabs, were processed in parallel to monitor background contamination. Environmental conditions (15–18 °C temperature, 82–84% relative humidity) were logged for each firing, and times between detonation, re-entry, and sampling were standardised (15 min. Safety interval).

2.2.1. Chemical-IED replica design

Experimental explosive devices were designed to simulate fragment contamination rather than a bulk liquid release, as fragmentary dispersal is more likely to result in widespread secondary contamination, thereby increasing the number and diversity of contaminated

evidential matrices encountered during post-incident forensic recovery when compared with uniform liquid deposition [20,55]. In addition, the devices were designed to reflect surfaces and items likely used in a real-world event [57]. This selection of materials allows for a realistic assessment of residue deposition across a range of matrix types encountered in operational scenarios. Each device comprised an aluminium container (80 mm diameter, 54 mm height) encasing a 10 g military-grade plastic explosive (PE-8) main charge initiated by a commercial L2A2 electric detonator. PE-8, a British insensitive, RDX-based plastic explosive with an oxygen balance of -21.6% , is primarily used by the military and for commercial demolition operations [58]. It is more energetic than 2,4,6 trinitrotoluene (TNT), but less toxic than other modern alternatives and provides a high level of safety [59]. To allow for detonator placement, a 7 mm hole was punched into the centre of each container lid. Forty 6 mm ball bearings were used to generate fragmentation. These were individually prepared using three deposition methods, as described in Section 2.2.2. To reduce immediate simulant degradation during detonation, the explosive charge was physically separated from the simulant-coated ball bearings. Data from triplicate firings and multiple swab or fragment samples were used to calculate mean residue recovery and standard deviations.

2.2.2. Deposition methods

Three deposition methods (Fig. 3) were evaluated to assess residue transfer and retention on different fragment matrices. Cotton wool (Superdrug, London, UK) and a 50:50 cotton–polyester blend (Colour Match, Seattle, USA) were selected because they are common and readily available materials. Cotton wool was chosen for its high absorbency, while the cotton–polyester bedsheet fabric was included to enable comparison of different adhesion geometries and their influence on simulant retention. In Method A, individual ball bearings were wrapped with 20×20 mm squares of 50:50 cotton–polyester fabric and secured using double-sided adhesive tape (Hannon, Walsall, UK). In Method B, 20×20 mm fabric squares were affixed flat to each ball bearing using a small amount of cyanoacrylate adhesive (UHU GmbH & Co, Buhl, Germany). In Method C, ball bearings were first attached to the container using double-sided adhesive tape, after which 10 cm strips of cotton wool were wrapped around the exterior of the container. Following assembly, the exterior of each container with attached ball bearings was submerged in approximately 2 cm^2 of 100 mg/L simulant solution to ensure complete coating of all wrapped ball bearings, before the IED replicas were carefully sealed in polyethylene sleeves for transportation to the containment building. Each deposition method was tested using three independent devices ($n = 3$). Method A was

Table 1

Summary of detonation conditions characterised by the charge size, simulant, distance to the target, and deposition method used.

Firing no.	Conditions
1	Charge size (PE8) = 20 g Simulant = none Strawboard distance = 2 m
2	Charge size (PE8) = 10 g Simulant = none Strawboard distance = 2 m
3–5	Charge size (PE8) = 10 g Simulant = methyl salicylate Strawboard distance = 1 m Wrapped ball bearings in 50:50 cotton- polyester fabric
6–8	Charge size (PE8) = 10 g Simulant = methyl salicylate Strawboard distance = 1 m Cotton wool wrapped ball bearings 10 g charge
9–11	Simulant = methyl salicylate Strawboard distance = 1 m Flat wrapping of ball bearing with 50:50 cotton- polyester fabric 10 g charge
12–14	Simulant = malathion MDF board distance = 1 m Wrapped ball bearings in 50:50 cotton- polyester fabric



Fig. 3. Diagram of all three deposition methods and blank IED.

additionally evaluated using malathion, whereas methyl salicylate was tested across all three methods.

2.3. Sample collection and handling

Following a 15-min safety interval, in situ sampling of fragments—including fabric, ball bearings, plastic debris from the polyethylene sleeve, and container remnants—was conducted. Samples were collected from the area between the blast-resistant block and the target. Additionally, the walls of the containment building were inspected for fragments. Each fragment was individually collected using tweezers and placed into labelled glass vials, in accordance with AEP-66 guidance [14]. To investigate the applicability of composite sampling in post-blast scenarios, matrices adhering to one another were not separated intentionally. Instead, they were combined into a single bulk sample, allowing evaluation of composite sampling while reducing analytical time, material use, and overall processing costs compared to analysing each matrix individually [60–64]. Impact points on the strawboard were swabbed at three identified penetration sites per target using cotton-tipped swabs pre-wetted with acetonitrile. Swab and wipe samples are unique among solid evidence because their forensic significance comes mainly from the transfer process, not from the bulk matrix itself [49]. Furthermore, cotton swabs were selected due to their common use by military teams [14,49]. Swabs and fragments were stored at 4 °C and extracted within one week to prevent analyte degradation.

2.4. Extraction conditions

Following collection, all samples, including swabs and fragments, were subjected to solvent-based extraction using acetonitrile. Acetonitrile is an organic, polar, aprotic solvent that is miscible with water and most organic solvents [65]. Its low viscosity enables improved surface wetting and penetration into surface irregularities compared with higher-viscosity solvents. In addition, acetonitrile is compatible with HPLC analysis and reduces chromatographic interferences [50]. Importantly, malathion and methyl salicylate are both readily soluble in acetonitrile [54]. To ensure procedural consistency, acetonitrile was used as both the wetting and extraction solvent for all fragment and

swab extraction samples [49]. Each sample was placed in a clean glass vial with 4 mL of HPLC-grade acetonitrile. This volume was selected to ensure full submersion of the swab tip and fragment while limiting dilution of recovered residues [51]. Following solvent addition, each vial was agitated on an orbital shaker (Cole-Parmer Stuart SSL1, Chelmsford, UK) at 200 rpm for 30 min at ambient temperature. Shaking generally achieves more reproducible results than sonication [48]. After shaking, the vials were then allowed to stand briefly to allow particulates to settle. The resulting extract was filtered directly through a 0.22 µm PTFE syringe filter (Fisher Scientific, Loughborough, UK) into a labelled HPLC vial using a 5 mL single-use plastic syringe. Extracts were stored at 4 °C prior to chromatographic analysis. Procedural blanks, including clean fragments, solvent blanks, and solvent-only swabs, were included in every extraction batch to monitor background contamination and potential cross-contamination. Extraction efficiency was assessed by conducting spike-recovery experiments by spiking 75 µL (7.5 µg) of each 100 µg/mL simulant solution onto three clean samples of each matrix (swab, plastic, cotton–polyester fabric, cotton wool, container, and ball bearings), followed by extraction with 4 mL of acetonitrile at 200 rpm for 30 min at ambient temperature. Each matrix was analysed in triplicate, and mean extraction efficiencies and associated standard deviations were calculated. Positive (analyte and solvent) and negative controls (matrix and solvent) were analysed concurrently to assess spike recovery and matrix effects.

2.5. Chromatographic analysis

Chromatographic analysis was performed using RP- HPLC on a Waters 2695 system equipped with a Waters 996 photodiode array detector (Milford, USA). Separation was achieved using a ZORBAX Eclipse Plus C-18 capillary column (4.6 × 150 mm, 3.5 µm; Agilent Technologies, Santa Clara, USA). The HPLC conditions used for analysis are recorded in Table 2. This analytical method was designed for the targeted quantification of the parent analytes, malathion and methyl salicylate. Degradation products were not investigated, and no co-elution or interfering signals were observed at the analyte retention times.

The LOD and LOQ were calculated based on the standard deviation of the response (σ) and the slope (S) of the calibration curve, using the

Table 2

Summary of HPLC conditions for each simulant.

Simulant	Mobile phase composition	Flow rate (mL/min)	Injection volume (μL)	Temperature (°C)	Detection wavelength (nm)	Retention time (min)
Methyl salicylate	Methanol: HPLC-grade water/0.1% formic acid (65/35, V/V)	0.5	10	35 ± 5	305	10.4
Malathion	Acetonitrile: HPLC grade water/0.1% formic acid (50/50, V/V)	1	10	35 ± 5	210	13

Calibration curves for both simulants were constructed in triplicate over a concentration range of 0.5–5 mg/L. Calibration standards were prepared by serial dilution from a gravimetrically manufactured 100 mg/L stock solution in HPLC-grade acetonitrile. The performance of the analytical method was evaluated in accordance with ICH Q2 (R1) guidelines for linearity, repeatability, limit of detection (LOD), and limit of quantification (LOQ) [66]. Linearity was assessed across 0.5–5 mg/L for both methyl salicylate and malathion (Table 3).

Table 3

Linearity measurements across the averages of three measurements taken for each simulant at specified detection wavelengths.

Simulant	Wavelength	Regression equation	R ²	Linear range (mg/L)
Methyl salicylate	305 nm	y = 563.79x - 104.36	0.9939	0.5–5
Malathion	210 nm	y = 1512.7x - 668.96	0.9925	0.5–5

ICH-recommended formulas:

$$LOD = \frac{3.3 \cdot \sigma}{S}, LOQ = \frac{10 \cdot \sigma}{S}$$

The LOD for malathion was 0.47 mg/L, whereas that for methyl salicylate was 0.3 mg/L. The LOQ for malathion was 1.43 mg/L, and for methyl salicylate, 0.9 mg/L (Table 4). Repeatability reflects the closeness of agreement between a series of measurements obtained under the same operating conditions over a short interval of time. For chromatographic methods, repeatability is typically assessed either by performing at least six replicate injections of a single sample solution at 100% of the test concentration or by evaluating nine determinations across the specified range of the method [66]. Results are expressed as the percentage relative standard deviation (%RSD) [66,67]. Although ICH does not prescribe a specific numerical acceptance limit for %RSD, industry practice and several methodological guides suggest that a %RSD of ≤2% is generally acceptable for repeatability in HPLC assay methods [66,68]. This threshold is widely recognised as demonstrating adequate precision for quantitative determination of the main analyte. Slightly higher %RSD values may be acceptable for impurity or trace-level determinations, depending on method sensitivity and concentration level [66,68] (Table 5).

2.6. Statistical analysis

Residue detection post-blast was treated as a binary outcome (detected vs. not detected). Binary logistic regression was used to assess the effects of sample matrix, simulant type, and deposition method on the likelihood of residue detection. All predictors were included as categorical variables, allowing each category to be statistically compared against a baseline category to quantify differences in the likelihood of residue detection. Binary logistic regression was selected in preference to analysis of variance (ANOVA) because it accommodates unequal group sizes arising from post-blast sample survivability. In addition, ANOVA was inappropriate because the data were left-skewed

Table 4

Summary of LOD and LOQ for each simulant at specific detection wavelengths.

Simulant	Wavelength	LOD (mg/L)	LOQ (mg/L)
Methyl salicylate	305 nm	0.30	0.90
Malathion	210 nm	0.47	1.43

Table 5

Repeatability measurements for methyl salicylate and malathion across all standards.

Concentration (mg/L)	%RSD Methyl salicylate	%RSD Malathion
0.5	2.5	5.3
1	1.7	0.7
1.5	0.7	3.6
2	0.6	3.2
2.5	2.7	2.7
3	1.0	1.6
4	2.4	2.0
5	0.6	2.0

and did not follow a normal distribution, thereby violating ANOVA assumptions [69]. It is important to note that this approach reduces continuous concentration data to a binary outcome, which reduces sensitivity and obscures variation in recovery magnitude. Alternative approaches, such as generalised linear models (GLMs) with non-normal distributions (e.g., gamma or log-normal) or non-parametric comparisons (e.g., Kruskal-Wallis or Mann-Whitney tests), could model continuous concentrations directly; however, these methods may be less robust in the presence of zero-inflation and measurements near the detection limit [70]. Consequently, logistic regression was deemed most appropriate for the detection-focused objectives of this study. All analyses were performed using Minitab, LLC software (State College, USA), with results reported as odds ratios with 95% confidence intervals.

3. Results and discussion

3.1. Solvent selection and extraction efficiency

Rather than optimising solvent selection, this study adopts extraction conditions established in prior forensic and environmental literature. The VERIFIN Blue Book explicitly states that organic extraction should be prioritised over aqueous extraction to prevent hydrolysis or degradation of the CWAs [27]. However, AEP-66 recommends the use of water or acetone as a wetting solvent, partially contradicting the previous recommendations to minimise degradation through hydrolysis [14]. A further consideration concerns the use of polar versus non-polar solvents. For example, some studies recommend non-polar solvents such as hexane, while others recommend polar solvents such as acetonitrile [48,50]. Other, more aggressive solvents commonly cited for swab-based extractions are acetone and isopropyl alcohol [14,27,48,71]. While dichloromethane is the extraction solvent recommended by the OPCW, its high volatility and toxicity render it unsuitable for use in this study [72]. Instead, acetonitrile was selected, supported by evidence from two independent studies identifying it as the most effective solvent for extractions of wipes/swabs contaminated with a range of CWAs and simulants [50,51]. The extraction efficiency of a solvent or solvent system is defined as the ratio of the amount of analyte(s) extracted to the total amount of analyte(s) present in a given sample. Under this definition, potential losses occurring during subsequent steps, such as

sample cleanup, solvent evaporation, or solvent exchange, are not taken into account. Extraction yield is influenced by several parameters, including extraction time, extraction temperature, agitation, and the nature of the extraction solvent [73]. Under the conditions tested, extraction efficiency ranged from 95% to 72% for malathion residues, with cotton wool samples exhibiting the highest extraction efficiency (Fig. 4). By comparison, for methyl salicylate residues, extraction efficiency ranged from 87% to 36%, with ball bearings exhibiting the highest and plastic the lowest efficiency. The low recovery of methyl salicylate is most likely attributed to the loss of analyte during the transfer of the spiked plastic into the extraction vial. Because spike-recovery experiments demonstrated quantitative and reproducible recovery across all substrates, no correction factors were applied (Fig. 4). Furthermore, no significant matrix effects were observed in the negative control samples for each matrix, supporting the reliability of quantitative comparisons between substrates.

3.2. Effect of deposition methods on residue retention

While this study does not directly measure surface interactions or thermal degradation pathways, interpretations are consistent with established physicochemical principles. The proposed mechanisms should therefore be interpreted as plausible explanations rather than definitive causal confirmation. Post-blast residue retention was strongly influenced by the deposition geometry, with configurations that increased surface area and confinement yielding greater detection frequencies across matrices (Fig. 5). Method C (cotton wool-wrapped deposition) produced the highest proportion of non-detect (ND) samples (38%; Fig. 5d), despite its higher absorbency and greater initial uptake. In contrast, 21% of samples from Method A (wrapped deposition) and only 9% from Method B (flat-wrapped deposition) fell into the ND category, suggesting substantially improved residue recoverability when the 50:50 cotton–polyester fabric was used instead of cotton wool.

The higher residue recovery of Methods A and B is linked to fibre composition. Polyester exhibits higher thermal resistance than cotton, with a melting point of approximately 250 °C and ignition at 440 °C, whereas cotton ignites at 215 °C [74]. As a result, polyester-containing fabrics are more likely to withstand the elevated temperatures associated with explosive events, reducing fibre degradation and subsequent residue loss post-detonation, consistent with the higher recoveries observed [75]. Consequently, cotton wool-based deposition (Method C) resulted in markedly lower overall residue concentrations (0.30–4.46 mg/L; Fig. 6d).

Attachment geometry further altered residue retention. Samples prepared using configurations that increased surface area (Method B: flat-wrapped) exhibited higher residue detection frequencies across multiple matrices, particularly for fabric and ball bearings, although most concentrations remained low (Fig. 5c). A larger surface area directly increases the amount of absorbed residue, leading to more

retention.

Binary logistic regression further supported these observations. Method B (flat-wrapped deposition) showed markedly higher odds of residue detection compared with Method C (cotton wool-wrapped) (OR = 11.54, CI 2.95–45.15). By contrast, Method A (wrapped deposition) showed increased odds relative to Method C (cotton wool-wrapped deposition; OR = 2.21), although this difference was not statistically significant. Comparison of Methods A (wrapped deposition) and B (flat-wrapped deposition) yielded an odds ratio of 0.2, with a confidence interval excluding 1, indicating that samples from Method A were significantly less likely to retain residues than flat-wrapped samples. Collectively, these results demonstrate that both matrix composition and attachment geometry contribute to retention probability (cotton–polyester > cotton wool; flat-wrapped > wrapped > cotton wool-wrapped).

While these findings indicate that flat-wrapped configurations promote enhanced residue retention, during simulant application, partial detachment of fabric from ball bearings was observed. [42]. This was likely due to solvent-adhesive interaction, which may have further contributed to residue transfer dynamics. Overall, the data support geometry-controlled transport rather than intrinsic material chemistry alone as the dominant mechanism for residue persistence following detonation.

3.3. Matrix-dependent retention

Evaluation across all sample matrices and deposition configurations indicated that fabric, container fragments, and composite samples retained the highest concentrations of simulant residues (Fig. 6). While the bulk of samples fell between LOD and LOQ, some fabric, container, and plastic samples exceeded the LOQ.

Container fragments consistently exhibited elevated residue concentrations, predominantly concentrated in the 1–1.5 mg/L range, and were primarily attributed to malathion residues (Fig. 6b; Fig. 7). Fifty per cent of composite samples exceeded the LOQ, compared with 31% of fabric and container samples (Fig. 6). Composite samples containing fabric consistently yielded the highest residue levels, confirming the fabric's dominant contribution to methyl salicylate retention. In contrast, composite samples lacking fabric frequently produced no detectable results, highlighting the dependence of recoverability on constituent materials.

Swab recovery was variable, highlighting the inherent challenges in sampling porous and heterogeneous surfaces. Notably, 70% of swabs recovered methyl salicylate within the LOD–LOQ range, whereas 66% of swabs returned no detectable malathion residues. Flat-wrapped fabric samples yielded quantifiable methyl salicylate residues in 67% of samples (Fig. 6c). Plastic fragments, ball bearings, and swabs retained quantifiable residues in 33%, 29%, and 25% of samples, respectively.

Across all detonations, 50% of plastic samples returned ND results, contradicting guidance in AEP-66, which outlines plastic as a favourable matrix for CWA residues (Fig. 7) [14]. This discrepancy underscores the importance of specifying polymer type, as polyester, also a plastic, outperformed naturally derived fibres such as cotton. Similarly, 43% of ball bearing samples were classified as ND, including over 90% of malathion samples, consistent with the low adhesion capacity of this metal surface. A further 43% of ball bearing samples, primarily attributed to methyl salicylate residue, fell between the LOD and LOQ. In contrast, 50% of container samples retained residues in the 1–2 mg/L range, with a further 25% in the 1.5–1 mg/L range.

Binary logistic regression confirmed significant matrix-dependent effects. Fabric and container samples exhibited significantly higher odds of residue detection relative to ball bearings (OR = 6.99 and 6.57, respectively). Composite samples were also associated with a higher odds ratio relative to ball bearings (OR = 10.46), although the wide confidence interval suggests substantial variability. In contrast, plastic and swab samples showed no statistically significant increases in residue

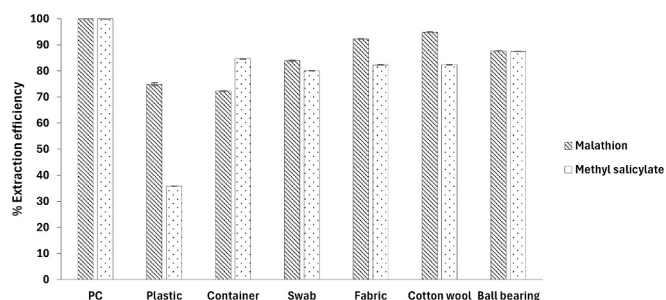


Fig. 4. Average extraction efficiency ($\pm$ standard deviation) across triplicates for all sample matrices, the positive control (PC), and both simulants. The PC represents a direct spike of each simulant into the extraction solvent (acetonitrile), providing a reference for maximum expected recovery.

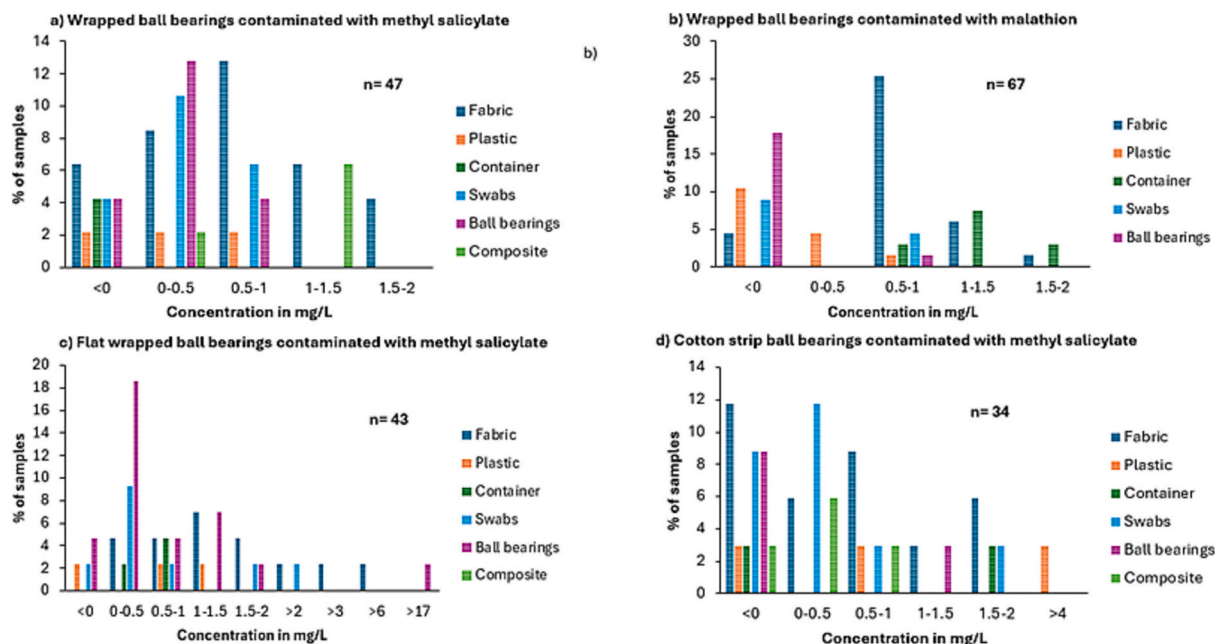


Fig. 5. Percentage distribution of measured concentrations (mg/L) for samples collected from fabric, plastic, container, swabs, ball bearings, and composite samples following post-blast recovery of wrapped ball bearings contaminated with methyl salicylate (a), wrapped ball bearings with malathion (b), flat-wrapped ball bearings with methyl salicylate (c), and cotton strip ball bearings with methyl salicylate (d). Sample size (n) is indicated for each experimental condition.

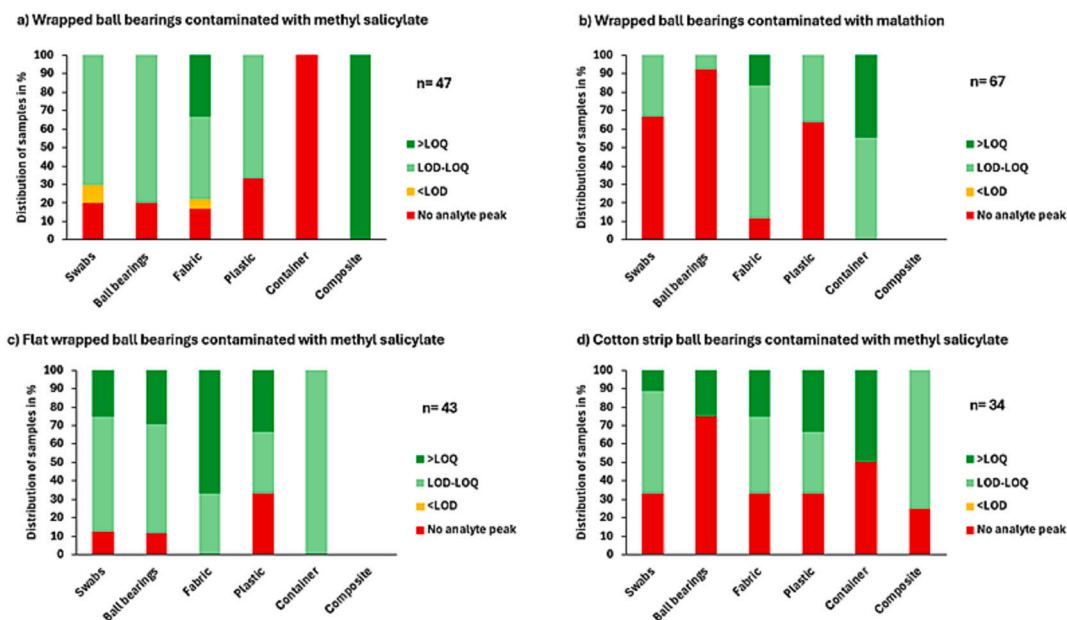


Fig. 6. Percentage distribution by detection category (>LOQ, LOD-LOQ, <LOD, and no analyte peak). of samples relative to the total number of samples collected for each sample type: swabs, ball bearings, fabric, plastic, container and composite samples. Graphs show wrapped ball bearings contaminated with methyl salicylate (a), wrapped ball bearings with malathion (b), flat-wrapped ball bearings with methyl salicylate (c), and cotton strip ball bearings with methyl salicylate (d). Bars represent the percentage of samples in each detection category. Sample size (n) is indicated for each experimental condition.

detection relative to ball bearings, and comparison with fabric demonstrated significantly lower odds of residue detection. Container fragments did not differ significantly from fabric. Comparisons involving composite samples with other matrices were statistically inconclusive due to the wide confidence intervals encompassing 1, reflecting high variability.

Overall, matrix-dependent retention reflects the combined influence of matrix structure and thermal behaviour under blast conditions, affecting adsorption, volatilisation, and persistence. While these

processes were not directly measured, the observed trends are consistent with these established principles. Porous, fibrous and less flammable materials enhance retention due to delayed volatilisation, whereas smoother, non-porous surfaces primarily retain residue through weak, reversible interactions.

These findings suggest that combining composite and individual fragment analyses can improve reconstruction of contamination patterns and device configurations, while highlighting surface swabbing as a complementary but low-yield approach [14,49,55].

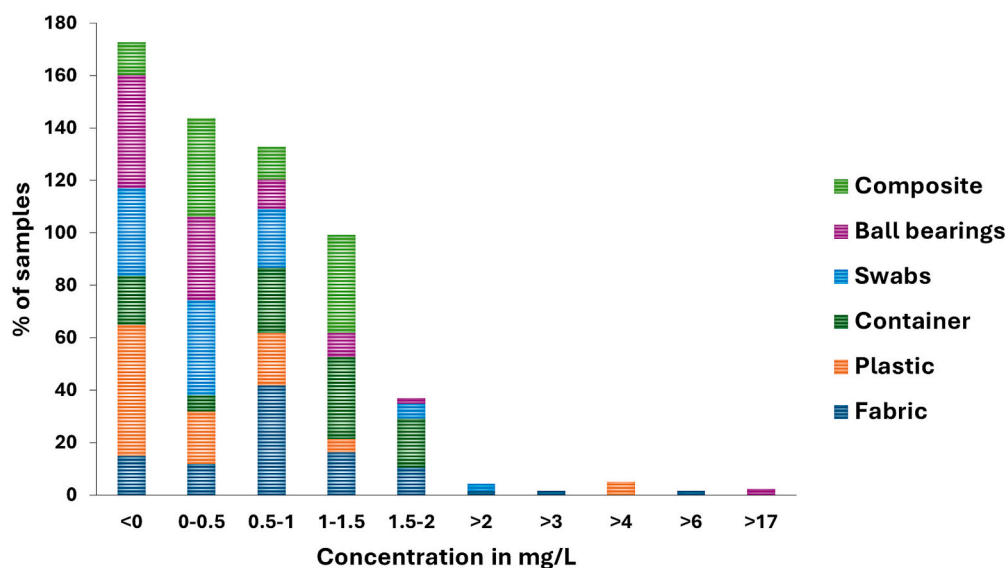


Fig. 7. Cumulative percentage distribution of samples by concentration range (mg/L) across each sample matrix. Each bar represents the total proportion of samples within a given concentration interval, with individual coloured segments indicating contributions from composite, ball bearing, swab, container, plastic and fabric samples.

3.4. Matrix-dependent retention influenced by simulant physicochemical properties

Under ambient conditions, malathion is typically more persistent than methyl salicylate, consistent with its lower volatility (0.00004 mmHg vs 0.03 mmHg for methyl salicylate) and higher density (1.208 g/mL vs 1.174 g/mL) [54]. However, this trend was not consistently observed following detonation. Although the odds ratio suggested slightly higher detection likelihood for methyl salicylate ($OR = 2.22$), the 95% confidence interval included 1, indicating no statistically significant difference. The larger dataset for methyl salicylate, resulting from testing multiple deposition methods compared with a single method for malathion, likely improved the estimate precision relative to malathion. Fabric consistently exhibited high retention for both simulants, with the most frequent concentrations observed in the 0.5–1 mg/L range. While this pattern was common for both compounds, a greater proportion of malathion samples occupied this concentration bracket (Fig. 8a). Cotton fibres are primarily composed of cellulose, a linear polysaccharide containing multiple hydroxyl groups, and polyester, a polymer connected by ester linkages, both support intermolecular interactions through hydrogen bonding, contributing to the fibre's hydrophilicity and ability to absorb [76]. Both Malathion, a phosphorodithioate, and methyl salicylate have lipophilic and polar functional groups that promote surface binding with organic-rich matrices like cotton-polyester fabric through intermolecular interactions, contributing to the elevated residue persistence observed [77,78].

Plastic bag samples retained methyl salicylate more effectively than malathion, with 33% of samples falling within the 0.5–1 mg/L range and a subset exceeding 4 mg/L (Fig. 8b). In contrast, container fragments exhibited significantly higher malathion retention, with most samples falling within the 1–1.5 mg/L range (Fig. 8c). Aluminium surfaces readily form polar oxide layers through oxidation, where aluminium atoms react with oxygen molecules in the environment (Al_2O_3), which promotes adsorption of organophosphorus compounds through intermolecular interactions, therefore enhancing residue persistence post-detonation [77]. Malathion's phosphorous likely formed stable bonds through π conjugation to the aluminium oxide [79]. Contrastingly, methyl salicylate was retained more frequently on ball bearings and swabs, with most samples falling within the 0–0.5 mg/L range. Notably, isolated high-concentration outliers were observed, including a ball

bearing sample exceeding 17 mg/L (Fig. 8d, e).

To guide matrix prioritisation in post-blast events, mean concentrations and standard deviations were calculated for both simulants using Method A, and across both simulants and deposition methods (Table 6). The resulting heat map (Table 6) visualises matrix-dependent retention, with mean concentrations colour-coded as green for values >0.8 mg/L, yellow for values >0.5 – 0.8 mg/L, and red for values ≤ 0.5 mg/L.

For Method A (wrapped configuration), mean concentrations of malathion on fabric samples were 0.81 mg/L compared with 1.13 mg/L for methyl salicylate. Container fragments exhibited an average malathion concentration of 1.22 mg/L, whereas the corresponding methyl salicylate mean concentration was 0.34 mg/L. Smooth matrices, such as ball bearings and plastic, retained minimal malathion residues, with mean values of <0.20 mg/L for both matrices. However, across all deposition methods, plastic and ball bearings retained mean methyl salicylate concentrations of 0.88 mg/L and 1.02 mg/L, respectively (Table 6). The higher average concentrations of methyl salicylate on plastic and ball bearings reflect the influence of deposition method (flat-wrapped vs wrapped vs cotton wool-wrapped), illustrating that both simulant physiochemistry and adhesion geometry govern persistence.

Across all matrix types, fabric retained the highest mean simulant concentration (1.01 mg/L), followed by container fragments (0.78 mg/L) (Table 6). Ball bearings, plastic, and swabs retained lower mean concentrations of 0.73 mg/L, 0.5 mg/L, and 0.44 mg/L, respectively. Persistence, defined as detectable concentration remaining post-detonation, therefore follows the order fabric $>$ container $>$ ball bearings $>$ plastic $>$ swabs. For methyl salicylate, persistence was highest on fabric samples and lowest on container fragments, with intermediate retention on plastic and swabs (fabric $>$ ball bearings $>$ plastic $>$ swabs $>$ container). By comparison, ball bearings, swabs and plastic retained the lowest malathion concentration, while container fragments and fabric retained the highest (container $>$ fabric $>$ plastic $>$ swabs $>$ ball bearings).

Across all matrices and both simulants, surface swabs consistently exhibited the lowest recovery, whereas bulk fragment collection captured higher residue levels. These findings highlight that the two sampling approaches, bulk fragment recovery and surface swabbing, target different aspects of residue deposition and retention. Consequently, they should be regarded as complementary rather than interchangeable, and their combined use can provide a more complete picture of contamination patterns when feasible [49].

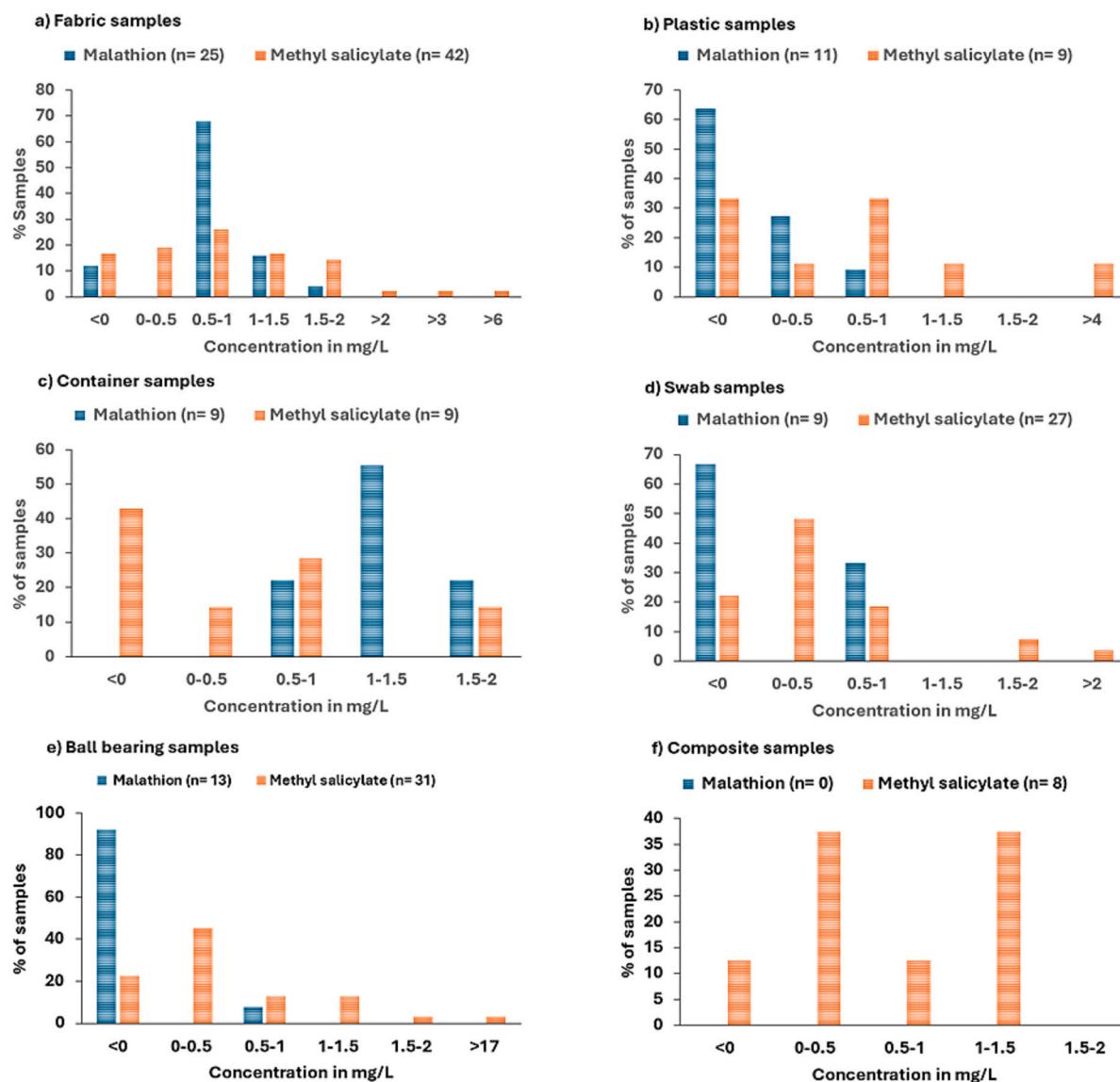


Fig. 8. Comparison of methyl salicylate (orange) and malathion (blue), concentration distribution across sample matrices, irrespective of deposition method. Graphs show the percentage of samples observed within each concentration range (mg/L) for each analyte, with total sample numbers (n) indicated in the legend. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 6

Heat map illustrating matrix-dependent retention in post-blast samples. Values represent mean concentrations, with standard deviations used to indicate matrix prioritisation for targeted sampling.

Average (mg/L) ± SD	Fabric	Plastic	Container	Swabs	Ball bearings
Methyl salicylate	1.13 ± 1.39	0.88 ± 1.55	0.34 ± 0.27	0.52 ± 0.57	1.02 ± 3.03
Malathion	0.81 ± 0.43	0.20 ± 0.28	1.22 ± 0.41	0.19 ± 0.28	0.05 ± 0.17
Combined	1.01 ± 1.14	0.50 ± 0.99	0.78 ± 0.56	0.44 ± 0.53	0.73 ± 2.57

Green: > 0.8 mg/L (High retention – priority matrix).

Yellow: > 0.5 to 0.8 mg/L (Moderate retention).

Red: ≤ 0.5 mg/L (Low retention).

3.5. Inferred post-detonation behaviour of CWAs

Inferences about the post-detonation behaviour of HD and VX can be

made, using the physicochemical analogy of methyl salicylate to HD and malathion to VX. In this context, physicochemical analogy refers to similarity in degradation pathways and physical properties of the

simulants at ambient temperatures to the agents, rather than identical functional group reactivity or toxicity. Accordingly, methyl salicylate and malathion cannot fully reproduce the degradation and nature of HD and VX. Inferences to real CWAs are therefore restricted to qualitative trends in thermal stability and decomposition onset.

Malathion is an organophosphorus (OP) molecule, like VX, and therefore shares key functional groups and degradation pathways. Malathion is miscible with most organic solvents, hydrolyses at pH 8, and decomposes at elevated temperatures [80]. VX exhibits a higher vapour pressure (0.000878 mmHg) than malathion at 25 °C (0.00004 mmHg), indicating greater volatility in ambient conditions (Table 7). However, boiling points suggest contrasting behaviour at elevated temperatures. Malathion boils at 156–157 °C, suggesting it may evaporate more rapidly than VX (298 °C) under rapid heating or detonation conditions, despite its lower ambient vapour pressure [80].

Computational studies predict VX to decompose completely at 477 °C in 2 s, with pyrolysis both kinetically and thermodynamically favoured across a temperature range of 327–727 °C [81]. In contrast, experimental observations suggest partial degradation of malathion initiates at 149 °C [82]. Under more extreme thermal exposure, malathion persistence decreases significantly. Only 11.93% malathion residues survived a temperature of 566 °C from thermally generated aerosol clouds [80]. Detonation environments can briefly reach temperatures up to 5000 K. However, RDX the principal explosive component of PE-8, starts decomposing at 170 °C, melts at 204 °C, and burns rather than detonates under many conditions [58,83,84]. As a result, detonations cause complex combinations rather than a uniform-high temperature exposure.

Furthermore, the thermal decomposition of OP has been studied for GB, GD and VX simulants. These studies identify pericyclic hydrogen transfer reactions via a 6-membered ring-structured transition state (TS) as the most common pathway under thermal conditions [85,86]. However, the 6-membered TS can only occur when the OP contains an ester

of phosphonate acid, ensuring adequate π -electron configuration, and a longer alcoholic side chain of the ester than a methyl group. Malathion does not satisfy the second requirement because its alcoholic side chain lacks the necessary alkane chain. Consequently, a less favourable pericyclic hydrogen transfer reaction with a 5 or 4-membered ring TS, requiring a higher activation energy, is more likely [85]. Compared to VX, this suggests malathion may undergo pericyclic hydrogen transfer less readily, potentially increasing its persistence under certain detonation conditions.

In contrast to OP compounds, methyl salicylate is an organic ester derived from salicylic acid, whereas HD contains both a sulfonyl and amino groups, making them chemically diverse [87,88]. Despite their chemical differences, both molecules primarily decompose via hydrolysis in the presence of water. HD and methyl salicylate also exhibit similar boiling points (215–217 °C and 220–224 °C, respectively) and comparable thermal stability (Table 7). At low environmental temperatures, HD undergoes a slow but continuous sulphonium-mediated ageing process. This pathway produces 1,4-dithiane, sesqui-mustard, and polymeric sulphides, which, together with incomplete hydrolysis, contribute to its long-term environmental persistence [89]. At temperatures below 400 °C, HD decomposes through combined intramolecular HCl elimination and C–S scission [90,91].

Upon temperature increase (600–800 °C), chlorine radicals accumulate, transitioning the dominant decomposition pathway to radical-driven pyrolysis, yielding rapid decomposition of HD within seconds at temperatures of 1000 °C [91]. Comparatively, methyl salicylate degradation is not dominated by radical chain reactions. Instead, at ambient temperatures, it undergoes stepwise oxidative loss via single-collision reactions, initiated primarily by hydroxyl radicals [92]. Under high temperatures, it is expected that hydrolysis will increase [31]. Degradation is not only governed by physicochemical properties such as volatility but also by molecular structure and the mechanistic accessibility of low-energy decomposition pathways.

From a hazard perspective, two significant risks emerge. First, contaminated fragments pose a transdermal exposure hazard. VX presents an extreme risk, with dermal toxicity occurring at quantities several orders of magnitude lower than vesicant agents such as HD. As a result, any unprotected skin contact is considered potentially fatal, with the LD₅₀ for undiluted liquid VX reported as 0.034 mg/kg (12h) and 0.029 mg/kg (24 h) [93]. HD vapours can penetrate clothing and damage underlying tissues, causing blistering of the skin and potentially leading to cancer later in life [94]. Second, the volatilised fraction poses an acute inhalation hazard, particularly in confined spaces. VX is among the most potent organophosphorous nerve agents, with early studies reporting an oral LD₅₀ of approximately 0.0023 mg/kg [95]. Subsequent toxicological assessments have estimated a higher oral LD₅₀ of 0.04 mg/kg body weight, while still indicating a substantial health risk associated with trace-level exposure [96]. The experimental observations demonstrate that post-blast fragmentation can distribute simulant at concentrations sufficient to mimic these risks, emphasising the importance of targeting high-retention matrices such as cotton–polyester fabric (for methyl salicylate) and aluminium container (for malathion) for residue detection, risk assessment, and post-event analysis.

4. Conclusion

This study provides the first systematic, quantitative investigation of CWA simulant retention and transfer following controlled explosive dissemination, demonstrating that blast-driven fragmentation modifies residue distribution and recoverability relative to non-detonative scenarios. Unlike earlier studies that focused primarily on quantitative analysis of explosive residues or qualitative assessments of dispersal, this research systematically examined how substrate properties and device-associated materials influence the capture and persistence of CWA simulants. Contaminant deposition geometry of the devices was shown to significantly influence persistence. Flat-wrapped fabric

Table 7
Physicochemical properties of the HD, methyl salicylate, VX and malathion retrieved from Pubchem after [54].

Physicochemical properties	HD	Methyl salicylate	VX	Malathion
Molecular weight	159.08 g/mol	152.15 g/mol	267.37 g/mol	330.4 g/mol
Solubility	Highly soluble in organic solvents	Highly soluble in organic solvents	Soluble in organic solvents	Miscible with many organic solvents
Density	1.2741 g/mL at 20 °C/4 °C (liquid) 1.338 g/mL at 13 °C (solid)	1.174 g/mL at 25 °C	1.0083 g/mL at 25 °C	1.2076 g/mL at 20 °C
Boiling point	215–217 °C	220–224 °C	298 °C	156–157 °C
Melting point	13–14 °C	–8.6 °C	–10 °C	3.85 °C
Toxicity	Acutely toxic	Irritant	Acutely toxic	Irritant, environmental hazard
Appearance	Oily yellow-brown liquid with garlic taste and mustard odour	Colourless yellowish or reddish liquid with the odour of wintergreen	Clear, colourless to amber-coloured liquid	Yellow to dark-brown liquid
Vapour pressure	0.11 mmHg at 25 °C	0.03 mmHg at 25 °C	0.000878 mmHg at 25 °C	0.00004 mmHg at 25 °C
Water solubility	609 mg/L at 25 °C	Slightly soluble	Moderately soluble	143 mg/L at 20 °C

configurations exhibited substantially greater residue retention than both wrapped and cotton-wool-based depositions, indicating that surface exposure and surface area play critical roles in moderating volatilisation, dispersal and post-blast persistence.

Clear matrix-dependent trends were also demonstrated, with porous and composite matrices, particularly cotton-polyester fabric and aluminium container fragments, consistently retaining higher residue compared to non-porous, smooth materials. Fabrics and container fragments, especially those associated with personal effects or device housings, therefore represent the highest-value matrices for residue recovery and should be prioritised during scene exploitation. These findings underscore the importance of considering matrix-dependent retention. Importantly, detectable residues on recovered fragments may remain at levels relevant to secondary exposure risk, underscoring the need for appropriate handling precautions during forensic and CBRN response operations. Comparatively, wet swabbing yielded the lowest recovery, highlighting the importance of complementary sampling approaches to maximise evidential recovery. When bulk extraction is not feasible due to operational constraints, such as safety concerns and equipment limitations, swabbing remains a useful sampling tool, albeit less effective. While direct extrapolation to CWAs must be treated cautiously, the physicochemical analogies employed suggest that vesicants such as HD may preferentially persist on porous matrices. In contrast, organophosphorous nerve agents with lower vapour pressures may be retained more effectively on metallic fragments.

Although an inherent limitation of this study is the use of an idealised blast configuration to enable controlled, reproducible comparisons, real-world IED events encompass a much broader range of geometries, charge sizes, and stand-off distances than those examined. Consequently, the absolute residue concentrations and detection frequencies reported here should not be interpreted as predictive for all scenarios. However, the controlled design allows isolation of key factors, particularly deposition geometry, matrix effects, and simulant physicochemical properties, governing relative retention trends. These relative effects are expected to persist across a wider range of configurations, even though their magnitude may vary with device design and explosive loading. This study enhances the understanding of post-detonation residue persistence and transfer by integrating controlled explosive testing with chemical and statistical analysis. It provides new mechanistic insight into matrix-dependent contamination patterns and delivers actionable guidance for improving forensic recovery, exposure assessment, and attribution following chemical-IED events.

CRediT authorship contribution statement

Sally Webb: Writing – review & editing, Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Frederic Coulon:** Writing – review & editing, Supervision, Funding acquisition. **David Crouch:** Writing – review & editing, Supervision. **Tracey Temple:** Writing – review & editing, Supervision, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data supporting this study are openly available from the Cranfield University repository at <https://doi.org/10.57996/cran.ceres-2820>.

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