Advanced Separation and Digital Strategies for Chemical Warfare Agent Mitigation

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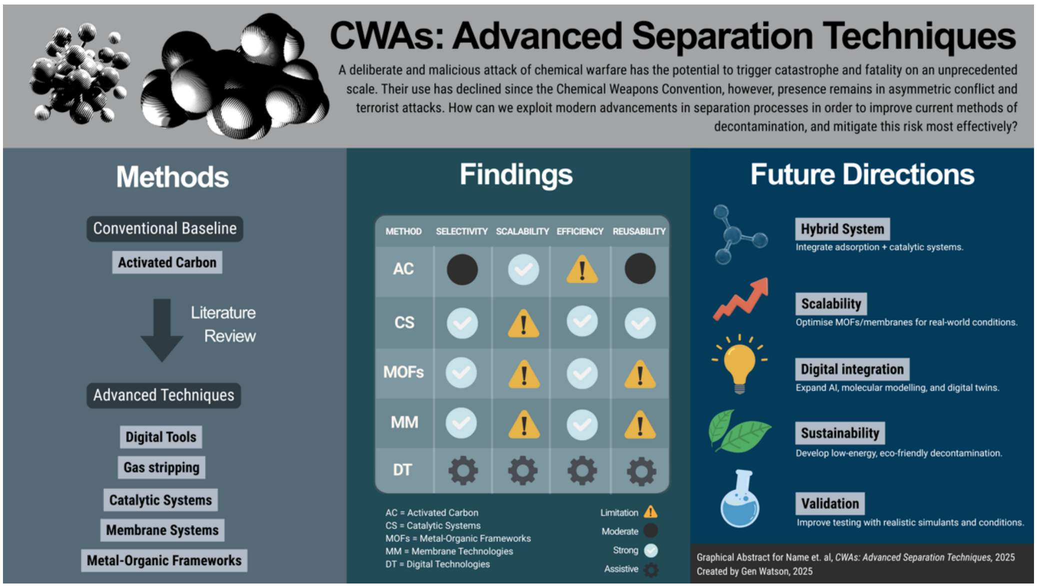
Graphical Abstract



Abstract

The persistent threat posed by chemical warfare agents (CWAs) arises from their acute toxicity, rapid environmental mobility, and long-lasting physiological and ecological impacts. Effective emergency response requires rapid and reliable decontamination strategies, and separation-based processes have emerged as critical tools for isolating, capturing, and neutralising these agents across air, water, and surface environments. This review synthesises recent advances in adsorption technologies, metal organic frameworks (MOFs), membrane filtration, gas stripping, and catalytic and oxidation-based approaches, highlighting how engineered materials and tuneable interfaces have enhanced selectivity and efficiency in CWA separation. Complementing these developments, molecular modelling, Monte Carlo and molecular dynamics simulations, high-throughput screening, and machine learning driven prediction have accelerated material discovery and deepened understanding of the structural and chemical factors governing CWA capture and degradation. Despite these advancements, persistent challenges including limited real agent validation, scalability constraints, fouling and material degradation, and uncertainties in computational models continue to restrict widespread field deployment. Emerging digital tools, such as AI assisted analytics, real-time data interpretation, and early-stage digital twin frameworks offer significant potential to strengthen situational awareness and operational readiness. Overall, continued progress will depend on integrating traditional separations with advanced computational and digital methods to develop robust, adaptive, and field ready decontamination systems capable of responding to evolving chemical threats.

Keywords: chemical warfare agents, adsorption, metal organic frameworks, membrane filtration, gas stripping, digital tools

1. Introduction

Terrorism utilising chemical warfare agents (CWAs) remains one of the most pervasive and escalating threats to global health and security.[1] Originally designed for military deployment, their indiscriminate impact has disproportionately harmed civilian populations.[2] CWAs - highly toxic chemicals used in World Wars I and II, the Cold War, and the Iran-Iraq War - caused millions of deaths, most during World War I.[2] The devastating persistence was exemplified in Halabja (1988), causing thousands of deaths and long-term disease.[3] International frameworks such as the Geneva Protocol (1925) and the Chemical Weapons Convention (CWC, 1993) prohibited their use. However, CWAs have re-emerged in recent conflicts, such as Douma (2018), and Salisbury (2018).[2]

The persistence of CWAs reveals their catastrophic potential. Advances in synthesis, the accessibility of precursors, and online information further exacerbate this risk.[4] CWAs exist as gases, liquids, aerosols, or powders, with diverse toxicological harms. Nerve agents inhibit neurotransmission, blister agents harm skin and lungs, and choking agents impair respiration.[4-8] Rapid toxicity and environmental stability enhance lethality, complicating medical countermeasures; no universal decontamination method exists.[4]

Traditional decontamination: chlorine neutralisation, water hydrolysis, and oxidation, are effective but limited.[4,9] In contrast, separation-based decontamination offers selective capture and immobilisation of CWAs. Activated carbon is widely used for adsorption, but it does not fully degrade all agents.[10] These limitations emphasise the need for advanced separation techniques with greater selectivity, reusability, and deployment potential. Emerging technologies, such as MOFs, membrane filtration, gas stripping, and catalytic systems offer greater selectivity, efficiency, and scalability.[11-14]

To address this persistent challenge, this review explores modern separation-based strategies for CWA decontamination. It first outlines the historical and contemporary scale of the problem, then surveys current and emerging separation techniques - including adsorption, metal-organic frameworks (MOFs), membrane filtration, and gas stripping. Finally, it discusses the major technological and practical gaps that remain.

Although 99% of declared stockpiles were destroyed under the CWC by 2023,[15] the threat of CWAs persists in asymmetric and terrorist contexts.[16] Recent incidents include Syrian government attacks (2013),[17] Iraq Islamic State assaults (2017),[17] and nearly 7,000 chemical events in Ukraine (2023-2025), causing thousands of injuries and deaths.[18] The impacts extend beyond mortality. Survivors suffer long-term respiratory, neurological, and psychological damage, creating humanitarian crises marked by forced migration, food insecurity, and loss of livelihoods. The 1988 Halabja attack exemplifies these consequences: 5000 deaths, mostly civilians, and decades of chronic illness among survivors.[3] CWAs also cause severe environmental damage. Their persistence in soil and water enables contamination lasting weeks to months.[19] Following World War II, 50,000 tons of CWAs were dumped in the Baltic Sea, releasing toxic by-products into sediments and marine food webs.[20] Research shows arsenic-containing degradation products in fish and ecosystem stress in marine organisms.[21,22] Similarly, soil contamination reduces microbial communities, disrupts nutrient cycling, and spreads through wind erosion, posing risks to ecosystems and human health for decades.[16]

Economic estimates are limited, but bioterrorism figures provide an analogue: events could cost USD $477.7 million - $26.2 billion per 100,000 exposed.[23] The 2001 US anthrax attacks cost $6 billion[24] in cleanup, healthcare, and productivity losses.[25] Comparably, CWAs would likely incur similar costs for decontamination, remediation, and loss of public trust.[26]

Recent literature has concentrated on the selective capture and degradation of CWAs using advanced separation materials and hybrid systems. MOFs stand out due to high surface area, tuneable pore structures, and catalysis: Huang et al. (2024) showed that MOF-polymer composites achieve near-complete detoxification of VX and mustard gas simulants.[13] Onodera et al. (2023) discussed a reactor that doubled removal efficiency compared to conventional stripping, suggesting potential for liquid-phase CWA decontamination.[14] Catalytic materials have 70-100% degradation efficiency but remain in early development phases, with Boddu et al. (2025) showing the need for scalable, low-energy systems.[12] Membrane filtration is highly suited for aqueous applications, and Bernardes et al. (2025) emphasises designs to improve selectivity and energy efficiency.[11] Activated carbon can be further enhanced: Verma et al. (2024) showed zirconium hydroxide integration increased adsorption and partial catalytic conversion of organophosphate simulants.[27]

Despite significant progress, several key challenges remain. Research still relies on simulants rather than live agents, scaling limits MOFs and membranes, and digital applications are constrained by data quality and computational resources. Moreover, conventional separations such as gas stripping and membrane filtration lack modern performance validation under realistic field conditions. These issues highlight the need to reassess how separation methods, catalytic reactivity, and digital tools can be integrated for safer, scalable, and sustainable CWA mitigation.

Consequently, this review addresses three overarching research questions. How can separation and catalytic strategies be engineered for high efficiency, scalability, and reusability in real-world environments? What are the comparative advantages and limitations of traditional (adsorption, gas stripping) and emerging (MOF, membrane technologies) separation platforms? How can computational and digital tools, such as machine learning, molecular models, and digital twins, be leveraged to accelerate material discovery, process optimisation, and risk reduction?

This review critically examines the advanced separation methodologies for CWA decontamination, focusing on MOFs, membrane filtration, gas stripping, and activated carbon, alongside their integration with catalytic and digital tools. While many studies demonstrate laboratory feasibility, the review emphasises the challenges of scaling to operational conditions.

This review includes 4 key objectives. Recent advancements and demonstrated performance of separation methods will be summarised. The critical challenges with scalability, selectivity, and long-term stability will be identified. It will evaluate integration opportunities with catalytic and digital technologies. Overall, this will highlight emerging directions that combine multiple separation or catalytic mechanisms to improve efficiency, sustainability, and deployability. This review does not address detection and sensor systems, real-time surveillance networks, or post-deployment forensic analysis, as these lie beyond the scope of separation-based decontamination.

2. State of the Art in Advanced Separation Strategies

2.1 Current Methodologies

The neutralisation of chemical warfare agents (CWAs) has been historically dominated by adsorption-based systems, with activated carbon forming the industrial baseline for protective technologies such as respirators, decontamination filters, and fixed-bed units.[8] The mechanism of such systems relies primarily on physical adsorption; however the use of impregnated carbons presents the added capacity of enhanced catalytic degradation, converting the captured CWAs into less toxic compounds.[28] Although highly scalable and cost-effective, conventional carbons are restricted by relatively low adsorption capacities, fragile catalytic sites, and limited structural tunability, thereby driving the need for more advanced separation and catalytic strategies to combat prevailing issues of CWA usage in conflict-prone environments.[29]

2.1.1 Activated Carbon (Conventional Baseline)

A study conducted by Yu et al. (2019) exemplifies the potential of engineered activated carbons through the synthesis of a porous carbon material from chitosan, a natural biopolymer, using potassium carbonate as the activating agent. The resulting carbon was tested against dimethyl methylphosphonate (DMMP), a commonly used nerve-agent simulant, where optimised carbons demonstrated an exceptionally high adsorption capacity of 432 mg g^{-1}, far exceeding many conventional carbons (50-150 mg g^{-1}).[30] Such a performance was attributed to controlled porosity, with higher activation ratios yielding surface areas greater than 1700 m^2 g^{-1}, large pore volumes, as well as to nitrogen-doping from the chitosan precursor, which facilitated strong polar interactions with DMMP molecules that accommodated their capture. These outcomes illustrate how biomass-derived activated carbons can be engineered to rival advanced materials such as metal–organic frameworks (MOFs) in terms of simulant capture, while offering advantages in cost, sustainability, and scalability.[31] However, this study only explored a single stimulant, where long-term stability or reusability under repeated cycling was not extensively characterised - a primary limitation. As such, further optimisation is required prior to extending the use of such materials from a laboratory environment to an industrial or field scale.[30]

2.1.2 Catalytic Materials as Alternatives to Carbon

To overcome the passivity of carbon adsorption, research has been increasingly focused on catalytic materials, including metal oxides, polyoxometalates, and metal clusters.[8] These systems possess large pores, high surface areas, and abundant active sites, enabling the direct chemical decomposition of CWAs - typically by disrupting the phosphorus-oxygen (P-O) bond in organophosphate nerve agents.[32] Unlike activated carbon, which merely sequesters toxic molecules, catalytic platforms can transform CWAs into benign products, thereby reducing risks of secondary contamination.[8]

A study by Kim et al. (2023) provides a compelling case of this approach through the development of a hybrid catalyst comprising MgO nanoparticles incorporated into mesoporous SBA-15 silica and covalently linked to graphene oxide (GO). Tested against the nerve agent simulant DMNP, the composite (MgO@SBA-15@GO) exhibited rapid degradation kinetics, achieving a half-life of 15 minutes under infrared (IR) LED irradiation, compared with ~ 45 minutes in the absence of IR exposure. This threefold improvement in reaction rate was attributed to the photothermal effect of GO, which locally elevated surface temperatures by 20-30 °C, thereby accelerating reaction kinetics without requiring external heating. Simultaneously, the SBA-15 support maintained a large pore volume (~ 0.8 cm^3 g^{-1}) and surface area exceeding 700 m^2 g^{-1}, stabilising MgO nanoparticles against aggregation and promoting efficient molecular diffusion to the active sites - factors that are essential in maintaining high reaction rates and reliable detoxification performance.[32]

Importantly, the composite retained over 90 % of its conversion efficiency after five consecutive reuse cycles, confirming its durability under repeated photothermal conditions.[32] Collectively, these results highlight how integrating oxide catalysis with ordered mesoporous frameworks and photothermal components can deliver self-sustaining detoxification systems that outperform adsorption only carbons, while simultaneously mitigating the stability and reusability challenges often encountered in MOF based catalysts.

2.1.3 Metal Organic Frameworks (MOFS)

MOFs represent another promising class of materials that combine extreme porosity with catalytic functionality.[33] Constructed from metal clusters that act as Lewis acid centres and multidentate organic ligands that provide structural flexibility, MOFs are capable of both adsorbing CWAs and catalysing their hydrolytic breakdown into non-toxic products. The chemical versatility of linkers further enables MOFs to serve as photocatalysts, converting light into chemical energy while expanding the operational window for targeted detoxification.[28]

Recent innovations in MOF development were reported by Oh et al. (2023),[34] who evaluated the zeolitic imidazolate framework-8 (ZIF-8), a subclass of MOFs, for its ability to adsorb the CWA simulants CEES and DMMP. By synthesising four different morphologies, cubic, rhombic dodecahedron, leaf-shaped and plate-shaped, the study systematically showed that adsorption efficiency is strongly dependent on morphology and surface charge. The cubic form of ZIF-8, which carried the highest positive surface charge (approximately +30 mV compared with +8 mV to +15 mV for other shapes), exhibited the greatest uptake, achieving adsorption capacities of approximately 620 mg g^{-1} for CEES and 480 mg g^{-1} for DMMP under comparable conditions. This characteristic was attributed to the favourable polar interactions between the positively charged MOF surface and the electron-rich moieties of the simulants. Notably, the cubic ZIF-8 retained over 90 % of its initial adsorption capacity after five reuse cycles, with minimal changes in BET surface area (< 3 % loss) and pore volume (< 5 % change), underscoring its cost-effectiveness and potential for waste minimisation in decontamination applications. These findings clearly highlight how precise control over ligand chemistry, surface charge and morphology can tailor MOFs for selective and highly efficient CWA-simulant detoxification.[35]

2.1.4 Gas Stripping

Gas stripping presents an alternative strategy for the capture and removal of volatile or semi-volatile CWAs from aqueous environments, operating through the transfer of contaminants from the liquid to the gas phase via a carrier gas stream. This mechanism is governed by Henry's Law, where the partial pressure difference between phases drives the volatilisation required for separation.[28]

The performance of gas stripping is strongly influenced by the choice of carrier gas: air and steam are frequently employed, with steam offering the advantage of heat-assisted volatilisation that reduces solubility and improves removal efficiency.[36] Conversely, inert gases (such as nitrogen) can be used where the prevention of oxidative side-reactions is required.[28] Stripping has been operationalised using conventional chemical engineering equipment, including packed towers, air-sparged hydrocyclones, and aeration basins, which facilitate efficient mass transfer through enhanced gas-liquid contact.

Unfortunately, there are minimal bench scale evaluations of the capacity of gas stripping in explicitly decontaminating CWAs, with MOFs and related technologies subsuming primary roles in overcoming CWA contamination instead. However, evaluations of liquid-gas phase transitions conducted by Asha et al. (2017)[37] confirm that simulants of CWAs with analogous properties such as CEES and DMMP readily partition into the vapour phase, thereby instating the suitability of stripping as a supporting separation method.[37] However, it is necessary to understand that simulants cannot fully replicate the complex physicochemical behaviour of true CWAs, particularly in terms of volatility, persistence, and interaction with real environmental matrices.[38,39] Thus, while gas stripping is validated at the conceptual level through simulant studies, further empirical research using safe but structurally analogous systems is essential to quantify its true efficiency and scalability in realistic emergency response scenarios.

Another key limitation of such a technique lies in the fact that CWAs are transferred rather than destroyed, necessitating additional downstream treatment to ensure safe neutralisation. However, the integration of this technology with advanced sorbent or catalytic systems addresses this challenge, where stripped vapours can be effectively polished using activated carbons or MOFs while catalytic reactors ensure the breakdown of volatile products into non-toxic compounds.[40,41] As such, the use of hybrid process trains combining stripping, adsorption, and catalytic degradation proves a viable procedure to effectuate decontamination, and have demonstrated high overall removal efficiencies and reduced environmental persistence of toxic agents.[28] Overall, although gas stripping is limited in its use individually, when incorporated within engineered multi-barrier treatment systems it holds significant promise as a scalable, front-line separation stage for comprehensive CWA decontamination.

2.1.5 Membrane Filtration

Membrane filtration, a well-established technology for wastewater treatment, is becoming an increasingly prevalent technology in CWA protection. Membrane filters behave as selective barriers, restricting the movement of particles and molecules through the membrane pores based on their sizes and chemical properties.[42] This mechanism is particularly valuable in the development of personal protective equipment (PPE) for CWAs where current methods of handling CWA exposure is by immediate detoxification through chemical reactions and catalysts, an approach effective only under certain conditions.[43] Studies on the blockage CWA permeation are limited but emerging and being realised in membrane filtration technologies, particularly polymer-based-membranes and nanomembranes.

2.1.5.1 Polymer Membranes

Amongst polymer-based-membranes, mixed membrane reactors (MMR), where solid phase catalysts are incorporated within the porous polymer matrix, have been particularly studied for CWA protection. The polymer matrix behaves as continuous diffusion nanochannels, enabling CWA movement through the matrix and in pathways that lead to the immobilised solid phase catalysts. Trapped by the catalysts within the membrane, CWAs are then catalytically degraded.[44]

Current research on MMR for CWA has predominately used MOFs as the solid phase catalyst, particularly Zirconium-based MOFs (Zr-MOF) for their high stability and efficient catalytic degradation of CWAs.[45] A study by Lee et al. (2020)[46] incorporating UiO-66 derivatives with a polysulfone (PSF) and testing against nerve agent simulant DMNP, highlights potential of MMR to refine PPE designs. High catalytic activities of MOF-808 enabled for 97% DMNP conversion on average into less toxic products of nitrophenol and DMPA. Followed by a washing process to regenerate the MMR, MOF-808 achieved 95% conversion. The ability for the MMR to regenerate and sustain high conversion performance emphasises the capacity for this technology to provide durable, reusable and, inevitably with multiple use, cost-effective protection - critical necessities for feasible high performing PPE against CWAs.[47]

Furthermore, MMR configuration can be tailored for different operational scales. Lee et al. (2020)[46] reported that both plate-in-frame (MMR-p) and hollow fibre (MMR-h) designs achieved near-complete DMNP degradation (97% and >97%, respectively). MMR-p offered high porosity and flux, compatible for small scale and surface-coating applications, while MMR-h's substantially larger surface to volume ratio (6000-8000 m^2/m^3, compared to 350-500 m^2/m^3 for MMR-p) is efficient for large scale, stockpiles of CWAs.[46] The structural variations demonstrate MMR capability to enable PPE to be adapted for diverse protection and decontamination situations. Polymer selection further reinforces this versatility. While Lee et al. (2020) opted for PSF for its high chemical and mechanical stability, Snider & Hill. (2023) utilised polymer PVDF, over poly(ethylene-co-vinyl acetate), with UiO-66 for its higher hydrophobicity provided 3.5 times more DMNP degradation.[44] Evidently, MMRs represent highly innovative separation technologies, where its structure and composition can be tuned for PPE optimisation against CWAs.

2.1.5.2 Nanomembranes

Nanomembranes represent the next stage in membrane technology for CWA protection, aiming to prevent CWA permeation for extended durations, rather than detoxify.[43] Within this emerging field, Graphene (GR) and Graphene Oxide (GO) nanosheet composite membranes have been the predominant focus, as the one-atom-thickness of these nanosheets enables for impermeability of small gases, when in a laminate structure, and yet high water-vapour moisture permeability (WVMP), mitigating heat stress and optimising PPE comfort.[47,48]

Kim et al. (2022)[43] constructed a GO and linear polyethylenimine (LPEI) membrane and found a 73% reduction in nerve simulant, dimethyl methylphosphonate (DMMP), penetration and whilst maintaining high water-vapour and nitrogen permeation of 67.91g/m^2 per day. Assembled by a spraying layer-by-layer method to control thickness and internal structure, the membrane's effective blockage owed to the sieving effect of GO nanosheets and the laminate structure, and the hydrogen bonding sites on LPEI that interacted with DMMP and limited its movement. Though there is incomplete blockage, the high (WVMP) and relatively simple method of construction (spraying layer-by-layer) is not to be overlooked and highlights the potential for GO based nanomembranes to balance breathability alongside protection and construction ease - essential design criteria for feasible, wearable PPE.[47]

A similar study by Song et al. (2022)[49] using also a multilayer design of GO laminate layer except on MOF-loaded membrane, obtained complete blockage for 2750, 1075, 176 min, and 7 days for CWAs ammonia, mustard, soman and dimethyl methyl phosphonate (DMMP), respectively, whilst retaining high moisture permeability, much above the required minimum of 1500-2000 g/m^2 per day. Both studies highlight that the barrier performance of nanomembranes not only depends on nanosheet arrangement, but also the multilayer design. Kim et al. (2022)[43] compared the LPEI/GO membrane with globular PEI/GO membrane and reported that the denser arrangement achieved by LPEI's linearity provided for smaller free voids (0.22nm) than the globular PEI (0.33nm), a more disorganised arrangement, ultimately leading to improved CWA blockage that was 72.65% greater. Song et al. (2022)[49] highlighted that the serial reinforcement of MOF-loaded layers is necessary for complete blockage as singular layers alone are inefficient. Collectively, these findings demonstrate that nanomembrane performance is governed by both nanosheet organisation and multi-layer reinforcement, and such integration establishes a design foundation for breathable, yet highly protective PPE against CWAs.

2.2 Integration of Emerging Technologies

2.2.1 Machine Learning

Machine learning (ML) is undeniably playing a significant role in advancing CWA separation research by accelerating material selection and performance prediction. The separation performance of MOFs depends strongly on compatibility of pore size, shape and chemical functionality with the particular

CWA.[50] As experimentally screening through thousands of possible MOFs is time consuming and hazardous to workers, Wang et al., 2023 combined a Computational-Ready Experimental MOF data base with high-throughput computational screening to train several ML models to efficiently predict the most effective MOF for CWA simulants. The best performing model, Extreme Gradient Boosting (XGB), achieved a high predictive R^2 of 0.80 ± 0.01 for simulant TSN, indicating potential for rapid and reliable identification of the best performing MOF material for CWAs. Furthermore, the ML analysis revealed key structure properties that enabled certain MOFs to outperform others, highlighting porosity, Henry's coefficient and hydrogen bonding. Ultimately, insights from Wang et al., 2023[50] underscores the integral role of ML in advancing MOF development for CWA separation, having the potential to enhance design decisions of MOFs based on feature importance reports, and expedite efficiency in accurately selecting the most suitable MOF to implement into PPE.

ML has also made a notable imprint on membrane-separation research by handling high dimensional chemical data based on membrane composition, properties and environment conditions, to accelerate the development of membranes that provide an optimised separation performance.[51] Though current ML work focuses mainly on gas separation and other non-CWA separation applications, these successes establish the foundation for the future integration of ML for CWA-specific membrane development as data resources specific to this application become more available.[51]

2.2.2 Molecular Models and Simulation Tools

Molecular modelling enables researchers to investigate how toxic compounds, such as nerve agent simulants (e.g., DMMP, CEES), interact with advanced materials like MOFs or graphene membranes before conducting hazardous experiments. This approach reduces experimental risk while saving both time and cost in the design of decontamination and separation systems.[52] Energetic modelling provides insights into CWA behaviour toward new materials. Although ab initio quantum methods are accurate, they are computationally expensive, promising the use of classical force fields such as UFF, DREIDING, and TraPPE for high throughput screening of MOFs. These methods, however, may overlook complex interactions at open metal centres. Monte Carlo simulations are often employed to predict adsorption isotherms and estimate uptake capacity, while Molecular Dynamics reveals diffusion and transport through pores, directly informing membrane design and personal protective equipment (PPE) filters. High-throughput screening further accelerates the evaluation of thousands of MOFs, enabling the discovery of structure property relationships such as pore size selectivity trends. More recently, genetic algorithms have been applied to evolve MOF structures with optimised uptake, suggesting that design principles from gas storage can be adapted to CWA capture.[52]

2.2.3 Digital Twins

Digital twins are dynamic virtual representations of physical assets, systems, or processes that mirror their real-world counterparts, enabling real time monitoring, analysis, and simulation.[53] In the chemical industry, they have become essential tools for enhancing operational efficiency, optimising processes, and supporting sustainable growth by integrating sensor data, historical information, and advanced analytics. The combination of AI, machine learning, IoT, big data analytics, and edge computing allows digital twins to provide deeper insights, predictive modelling, and faster decision making, transforming conventional approaches to chemical manufacturing. Beyond conventional operations, digital twins can also be applied to hazardous chemicals, including chemical warfare agents, to improve safety and risk management. By simulating processes, monitoring critical parameters in real time, and predicting potential failures, digital twins enable virtual testing of containment, decontamination, and mitigation strategies without exposing personnel to toxic substances. This reduces operational risk, strengthens environmental stewardship, and supports the efficient use of resources in high-hazard chemical environments.[54]

The defence sector can benefit greatly from Digital Twin technologies. By creating digital replicas of military assets, operations, and infrastructure, defence organisations can perform detailed simulations, optimise resources, and conduct predictive evaluations. This technology enables real-time monitoring of military equipment and facilities, supports proactive maintenance, and optimises logistics, offering substantial improvements in asset availability and efficiency. Digital Twins can be considered a foundational tool for protection against CWAs on which different additional technological instruments are implemented to enhance capabilities, for example by automating data flow, optimising data analytics, automating data flow, and extending functionality.[54]

Internet of Things (IoT) and Sensors: The current landscape of military Internet of Things (IoT) and sensor technologies is characterised by rapid advancement and broad integration into defence applications including CWAs. These technologies are central to enhancing operational capabilities, improving situational awareness, and providing critical operational and environmental data ensuring timely detection of a hazard whilst improving safety and risk management. In addition, Military IoT encompasses a network of interconnected devices that collect, exchange, and process data to facilitate real-time decision-making and strategic planning. Modern Sensor technologies in recent years are also capable of detecting a wide range of physical, chemical, and biological stimuli with high precision. Integrating sensors with AI and ML algorithms further amplifies their utility. Large datasets generated by these sensors can be processed in real time to identify patterns, predict equipment failures, and detect anomalies.[54]

Artificial Intelligence and Machine Learning Technologies: The combination of AI and ML driven technologies allows digital twins to analyse extensive data streams, facilitate pattern recognition, and improve situational awareness. ML methods such as deep learning, neutral networks and key algorithmic approaches including supervised and unsupervised learning, reinforcement and incremental learning, and anomaly detection, all of which enable systems to learn from historical data of the effects of CWAs (toxic chemicals, reactions, material behaviour) and adapt to evolving conditions, thus enabling faster decision making.[54]

Extended Reality (XR): Extended Reality (XR) comprises a spectrum of technologies. These include Augmented Reality (AR), which overlays digital content onto the real world, and Virtual Reality (VR), which immerses users in synthetic environments. XR solutions involve the replacement of traditional displays by laser-based projections or headsets which can integrate digital information into human perception. XR-based training has proven to be impactful in defence and can also be extended to their role in CWAs. In fact, XR has been implemented into use by the Netherlands Ministry of Defence. Operationally, XR can facilitate mission planning, remote assistance, and augmented operator field-of-view with labels or annotations, simplifying CWA detection and enhancing situational awareness. Given XR's ability to deliver intuitive, real-time interactions, it is exceptionally well suited for integration with digital twins.[54]

2.3 Comparative Analysis of Separation Methodologies

2.3.1 Adsorption

Adsorption remains one of the most widely used separation technologies due to cost effectiveness, and environmental friendliness. [50] However, traditional adsorbents such as activated carbon and metal oxides show weak interactions with CWAs, especially at low concentrations. Their amorphous nature, irregular pore sizes, and limited chemical tunability restrict selective adsorption performance.[50] Zeolites and activated carbon also suffer from limited capacity, low productivity, and high energy demands.[55]

To enhance performance, researchers have modified these materials with additives such as triethylene-diamine or metallic salts (Zn, Cu). However, because their pore structures remain amorphous and unpredictable, systematic performance improvements remain challenging. Recent studies suggest that MOFs offer solutions to these limitations.[56]

2.3.2 Metal Organic Frameworks

Compared to conventional porous materials, MOFs exhibit larger surface areas, higher porosities, and tuneable structures.[56] Despite these advantages, MOFs in powdered form are difficult to process, prone to agglomeration, and less efficient in real world applications. A promising alternative is the development of MOF gels, which feature gel networks with enhanced mass transfer, reduced diffusion barriers, and superior catalytic and adsorption activity. Beyond CWAs, MOF gels have also shown potential in addressing broader environmental challenges, including the remediation of heavy metals, toxic gases, organic pollutants, and fine particulate matter (PM2.5/PM10).[33]

2.3.3 Gas Stripping

Gas stripping operates on a simple principle of transferring contaminants from liquid to gas using carrier gases such as air, steam or inert gases. It is especially effective in the removal of volatile and semi-volatile CWAs like CEES and DMMP. However, the process requires solvents with specific properties (low volatility, high solubility), limiting its applicability.[57] Additionally, it is energy intensive, expensive, and often inefficient for large scale decontamination scenarios, as long processing times are required to handle high contaminant loads.[57]

2.3.4 Membrane Filtration

Membrane filtration has gained increasing attention as a selective barrier against CWAs. Advanced nanomaterial-based membranes, particularly those incorporating GO or hybrid composites, can block highly toxic vapours such as DMMP.[53] These membranes are lightweight, can be fabricated into ultrathin films, and have potential applications in protective apparel and filtration systems. Despite their promise, membrane technologies face challenges such as costly and energy intensive fabrication, reliance on hazardous synthesis routes, and degradation due to fouling, hardness, and prolonged exposure to harsh chemicals.[58]

While recent advances in metal-organic frameworks, AI driven predictive simulations, and digital twin technologies are rapidly changing the face of separation science, traditional separation techniques like gas stripping and adsorption continue to form integral parts of chemical decontamination systems. Modern computational methods such as molecular simulations and digital twins have further advanced understanding of adsorption mechanisms in MOFs, enabling predictive insights into pore structure, active site chemistry, and agent–material interactions.[28,33,50] Additionally, traditional methods such as gas stripping remain attractive due to their operational simplicity and scalability, despite well-documented limitations including solvent dependency and high energy consumption.[57,59] Similarly, membrane-based protection systems continue to offer strong selectivity and tunability for toxic vapour filtration, yet still face challenges related to fouling, long-term stability, and permeability–selectivity trade-offs.[11,43]

By integrating classical separations with advanced modelling and AI tools, researchers can now identify key structure property relationships that were previously inaccessible through experimentation alone. This combination bridges the gap between empirical design and predictive optimisation, improving process efficiency and safety in emergency decontamination scenarios. Nonetheless, practical implementation still faces barriers related to cost, energy requirements, and recyclability, highlighting the need for balanced hybrid solutions that leverage the robustness of traditional processes alongside the precision of modern technologies.

3. Challenges and Future Perspectives

3.1 Identified Challenges in Advanced Separation

Research into chemical warfare agent separations is shaped by several pressing challenges. One major issue is the limited availability of reliable data, since the extreme toxicity of CWAs necessitates the use of safer simulants such as DMMP for sarin or 2-CEES for mustard gas. While these analogues capture some of the relevant chemical properties, they do not fully replicate the reactivity of the real agents, creating gaps in accuracy and reliability.

Computational simulations and high throughput screening of materials such as metal organic frameworks (MOFs) have been used to address this limitation, yet these methods often yield invalid or inconsistent results.[56] Scalability is another hurdle, as MOFs are typically synthesised in powder form, which leads to handling difficulties, low volumetric efficiency, and pressure drop.[56] Although MOF based aerogels, which integrate the high porosity of aerogels with the adsorption and catalytic activity of MOFs, have been developed to address this, large scale synthesis, drying methods, and structural stability continue to limit practical applications.[60] A further challenge is the lack of up-to-date validation for conventional separations such as membrane filtration and gas stripping. Much of the available literature is based on earlier experimental studies, leaving uncertainty about their efficiency and relevance for modern emergency response contexts, as research focus has shifted toward advanced materials and digital strategies. Finally, the application of artificial intelligence (AI) in this domain faces difficulties due to the complexity of quantum systems, the need for high quality datasets, and the limitations of generalising across diverse chemical systems.[61] Since direct experimentation with CWAs is hazardous, data remain scarce, and simulations often require extensive computational resources.

Figure 1 presents a comparative overview of separation methodologies, highlighting their progression, and key limitations.

3.2 Critical role of Separation Strategies

Despite these obstacles, advanced separation techniques remain critical for developing effective responses to chemical threats. MOFs, with their ultra-high porosity, large surface area, structural stability, and tuneable pore size, have proven particularly effective for adsorption and degradation of CWAs. Compared with traditional materials such as activated carbon, enzymes, zeolites, and metal oxides, MOFs offer broader structural diversity, stronger adsorption capacity, more active sites, and faster reaction kinetics.[56] Complementing these materials, digital twins enable real time monitoring and virtual simulation of decontamination systems, allowing responders to test strategies before

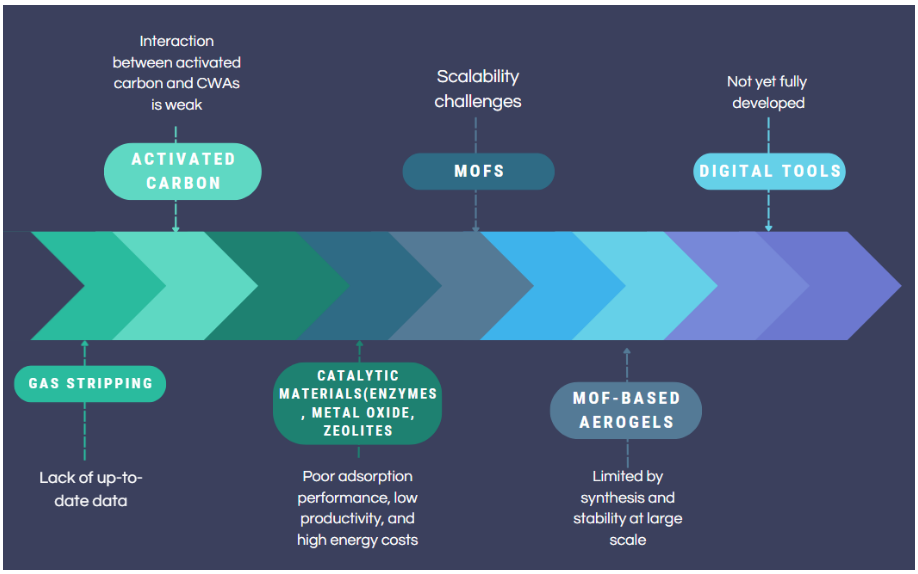


Figure 1: Evolution of separation and decontamination strategies for CWAs, with associated challenges.

deployment in the field, thereby improving decision making, reducing risk, and ensuring more efficient responses.[61] Similarly, AI and machine learning provide powerful predictive tools for identifying optimal separation materials and processes. Unlike traditional high throughput simulations, which are slow and often unreliable, machine learning can accelerate these processes by up to three orders of magnitude, while improving accuracy and guiding the identification of MOFs most suitable for decontamination.[56] Together, MOFs, AI, and digital twins represent promising directions that complement conventional approaches. While they do not fully overcome challenges, they provide safer, faster, and more adaptable tools that improve current research practices and pave the way for future advances in CWA mitigation.

3.3 Future Directions and Research Outlook

Looking forward, future research should aim to improve the balance between effectiveness and sustainability in separation methods, ensuring that new solutions do not introduce additional environmental hazards. The development of universal and eco-friendly approaches capable of neutralising CWAs across multiple forms, while minimising effluent production and energy consumption, will be critical. Greater emphasis should be placed on optimising existing techniques, combining complementary methods such as reactive membrane with gas stripping, and exploring novel materials and digital technologies. Ultimately, prioritising efficiency, safety, and environmental compatibility will be essential to ensure that separation strategies both protect human health and minimise ecological impact in the event of chemical emergencies.

4. Conclusion

Chemical warfare agents (CWAs) continue to pose a critical global threat due to their extreme toxicity, environmental persistence, and potential use in modern conflicts. Although international conventions prohibit their use, recent incidents underscore the ongoing need for rapid, efficient, and sustainable decontamination strategies. This review demonstrated that while conventional adsorption materials such as activated carbon are still relevant, newer separation-based technologies, including metal organic frameworks (MOFs), catalytic materials, membrane filtration, and gas stripping, offer superior selectivity, reusability, and structural tunability. MOFs and MMR show considerable potential for integrating adsorption and catalytic degradation within a single system, advancing the development of self-regenerating and environmentally responsible protective materials.

The integration of digital technologies further enhances these advancements. Machine learning accelerates the discovery and optimisation of novel materials, while molecular simulations and digital twins enable predictive performance assessment under controlled virtual conditions. However, significant challenges remain in scalability, cost effectiveness, data accessibility, and experimental validation with live agents. Future research should prioritise hybrid systems that combine multiple separation and catalytic processes, guided by artificial intelligence and life cycle sustainability principles.

Ultimately, the future of separation-based decontamination relies on translating laboratory scale innovations into robust, scalable, and sustainable technologies capable of mitigating the environmental and societal risks associated with chemical warfare agents.

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References

1 Ugwu, C. N. *et al.* Medical preparedness for bioterrorism and chemical warfare: A public health integration review. *Medicine (Baltimore)* **104**, e42289, doi:10.1097/md.0000000000042289 (2025).
2 Meng, W.-Q. *et al.* Fluorescent probes for the detection of chemical warfare agents. *Chemical Society Reviews* **52**, 601-662, doi:10.1039/D2CS00650B (2023).
3 Ahmed, D. R. & Al Diab Al Azzawi, M. The current global threat of weapons of mass destruction to humanity and public health. *Discover Public Health* **21**, 37, doi:10.1186/s12982-024-00161-6 (2024).
4 Labaška, M. *et al.* Neutralizing the threat: A comprehensive review of chemical warfare agent decontamination strategies. *Journal of Environmental Chemical Engineering* **12**, 114243, doi:10.1016/j.jece.2024.114243 (2024).
5 Dubey, A. *et al.* Role of flexible sensors for the electrochemical detection of organophosphate-based chemical warfare agents. *International Journal of Smart and Nano Materials* **15**, 502-533, doi:10.1080/19475411.2024.2385350 (2024).
6 Farhat, H. *et al.* Preparedness and emergency response strategies for chemical, biological, radiological and nuclear emergencies in disaster management: A qualitative systematic review. *Journal of Contingencies and Crisis Management* **32**, e12592, doi:10.1111/1468-5973.12592 (2024).
7 Thors, L. *et al.* Comparison of skin decontamination strategies in the initial operational response following chemical exposures. *Toxicology in Vitro* **87**, 105539, doi:10.1016/j.tiv.2022.105539 (2023).
8 Zhang, Y. & Tao, C.-A. Metal–Organic Framework Gels for Adsorption and Catalytic Detoxification of Chemical Warfare Agents: A Review. *Gels* **9** (2023).
9 Econdi, S. *et al.* Catalysis and decontamination: a versatile tool in the safe and sustainable degradation of chemical warfare agents. *The European Physical Journal Plus* **139**, 782, doi:10.1140/epjp/s13360-024-05582-5 (2024).
10 Saleem, J. *et al.* Life cycle assessment of high value activated carbon production based on mass and functional performance metrics. *Scientific Reports* **15**, 32797, doi:10.1038/s41598-025-16300-1 (2025).
11 Bernardes, A. F., Meng, Z., Campos, L. C. & Coppens, M.-O. Bio-inspired anti-fouling strategies for membrane-based separations. *Chemical Communications* **61**, 5064-5071, doi:10.1039/D4CC05149A (2025).
12 Boddu, V. M., Morales, J., Nadagouda, M. N., Oudejans, L. & Brooks, L. Thermophysical treatment technologies for chemical warfare agents sulfur mustard, sarin, and nerve agent VX – a review. *Environmental Science: Advances* **4**, 1538-1552, doi:10.1039/D5VA00071H (2025).
13 Huang, T., Chen, Q., Jiang, H. & Zhang, K. Research Progress in the Degradation of Chemical Warfare Agent Simulants Using Metal–Organic Frameworks. *Nanomaterials* **14** (2024).
14 Onodera, T., Takemura, Y., Aoki, M. & Syutsubo, K. Enhanced sulfide removal by gas stripping in a novel reactor for anaerobic wastewater treatment. *Water Science and Technology* **87**, 2223-2232, doi:10.2166/wst.2023.120 (2023).
15 Kelle, A. The CWC at 25: from verification of chemical-weapons destruction to attribution of their use. *The Nonproliferation Review* **28**, 319-336, doi:10.1080/10736700.2023.2180234 (2021).
16 Broomandi, P., Kim, J. R. & Rodríguez-Seijo, A. in *Sensing of Deadly Toxic Chemical Warfare Agents, Nerve Agent Simulants, and their Toxicological Aspects* (eds Sangita Das, Sabu Thomas, & Partha Pratim Das) 381-406 (Elsevier, 2023).
17 Chapman, G., Elbahtimy, H. & Martin, S. B. The Future of Chemical Weapons: Implications from the Syrian Civil War. *Security Studies* **27**, 704-733, doi:10.1080/09636412.2018.1483640 (2018).
18 Organisation for the Prohibition of Chemical Weapons (OPCW). Statement by the Delegation of Ukraine at the 108th Session of the OPCW Executive Council, Agenda Item 6(f) (OPCW, 2025)

19 Pampalakis, G. & Kostoudi, S. Chemical, Physical, and Toxicological Properties of V-Agents. *International Journal of Molecular Sciences* **24** (2023).

20 Vanninen, P. *et al.* Exposure status of sea-dumped chemical warfare agents in the Baltic Sea. *Marine Environmental Research* **161**, 105112, doi:10.1016/j.marenvres.2020.105112 (2020).

21 Lastumäki, A. *et al.* Biological effects of dumped chemical weapons in the Baltic Sea: A multi-biomarker study using caged mussels at the Bornholm main dumping site. *Marine Environmental Research* **161**, 105036, doi:10.1016/j.marenvres.2020.105036 (2020).

22 Polak-Juszczak, L. & Szlinder Richert, J. Arsenic speciation in fish from Baltic Sea close to chemical munitions dumpsites. *Chemosphere* **284**, 131326, doi:10.1016/j.chemosphere.2021.131326 (2021).

23 Kaufmann, A. F., Meltzer, M. I. & Schmid, G. P. The economic impact of a bioterrorist attack: are prevention and postattack intervention programs justifiable? *Emerg Infect Dis* **3**, 83-94, doi:10.3201/eid0302.970201 (1997).

24 Gosden, C. & Gardener, D. Weapons of mass destruction--threats and responses. *Bmj* **331**, 397-400, doi:10.1136/bmj.331.7513.397 (2005).

25 Schmitt, K. & Zacchia, N. A. Total Decontamination Cost of the Anthrax Letter Attacks. *Biosecurity and Bioterrorism: Biodefense Strategy, Practice, and Science* **10**, 98-107, doi:10.1089/bsp.2010.0053 (2012).

26 Schmitt, B. *et al.* Responding to a Small-scale Bioterrorist Anthrax Attack: Cost-effectiveness Analysis Comparing Preattack Vaccination With Postattack Antibiotic Treatment and Vaccination. *Archives of Internal Medicine* **167**, 655-662, doi:10.1001/archinte.167.7.655 (2007).

27 Verma, A. *et al.* Zirconium hydroxide-activated carbon hybrid material for chemical warfare agents detoxification: Implication of water and temperature. *Diamond and Related Materials* **150**, 111754, doi:10.1016/j.diamond.2024.111754 (2024).

28 Yang, J. *et al.* Advances in the adsorption and degradation of chemical warfare agents and simulants by Metal-organic frameworks. *Coordination Chemistry Reviews* **493**, 215289, doi:10.1016/j.ccr.2023.215289 (2023).

29 Claudot, J., Soubeyrand-Lenoir, E. & Maurin, G. Competitive adsorption of water and chemical warfare agents on transition metal embedded graphene. *Applied Surface Science* **551**, 149433, doi:10.1016/j.apsusc.2021.149433 (2021).

30 Yu, H. *et al.* Chitosan-Derived Porous Activated Carbon for the Removal of the Chemical Warfare Agent Simulant Dimethyl Methylphosphonate. *Nanomaterials* **9**, 12, doi:10.3390/nano9121703 (2019).

31 Kulkarni, H., Bari, C., Mukherjee, S., Gajera, P. & Sethia, G. Waste biomass-derived activated carbons for selective oxygen adsorption. *Carbon Trends* **17**, 100398, doi:10.1016/j.cartre.2024.100398 (2024).

32 Kim, Y. J., Heo, S. Y., Jang, W. J. & Lee, S. J. Metal oxide composites for detoxification of chemical warfare agent (CWA) simulant with enhanced catalytic activity under IR irradiation. *Microporous and Mesoporous Materials* **356**, 112588, doi:10.1016/j.micromeso.2023.112588 (2023).

33 Gao, M. *et al.* Adsorption of chemical warfare agents and their simulants by metal-organic frameworks: GCMC and DFT studies. *Journal of Environmental Chemical Engineering* **13**, 116628, doi:10.1016/j.jece.2025.116628 (2025).

34 Oh, S., Lee, S., Lee, G. & Oh, M. Enhanced adsorption capacity of ZIF-8 for chemical warfare agent simulants caused by its morphology and surface charge. *Sci Rep* **13**, 12250, doi:10.1038/s41598-023-39507-6 (2023).

35 Łuczak, J. *et al.* Morphology control through the synthesis of metal-organic frameworks. *Advances in Colloid and Interface Science* **314**, 102864, doi:10.1016/j.cis.2023.102864 (2023).

36 Karthick, C. & Nanthagopal, K. A comprehensive review on ecological approaches of waste to wealth strategies for production of sustainable biobutanol and its suitability in automotive applications. *Energy Conversion and Management* **239**, 114219, doi:10.1016/j.enconman.2021.114219 (2021).

37 Asha, P., Sinha, M. & Mandal, S. Effective removal of chemical warfare agent simulants using water stable metal–organic frameworks: mechanistic study and structure–property correlation. *RSC Advances* **7**, 6691-6696, doi:10.1039/C6RA28131A (2017).

38 Tasić, G., Ćurčić, M. & Perović, I. COMPARATIVE ANALYSIS OF PHYSICOCHEMICAL CHARACTERISTICS OF CHEMICAL WARFARE AGENTS AND THEIR SIMULANTS. in Thematic Conference Proceedings of International Significance: XII International Scientific Conference “Archibald Reiss Days” (eds. Milojević, B. et al.) 337–348 (University of Criminal Investigation and Police Studies, Belgrade, 2022). Available at https://www.researchgate.net/publication/365776465_COMPARATIVE_ANALYSIS_OF_PHYSICOCHEMICAL_CHARACTERISTICS_OF_CHEMICAL_WARFARE_AGENTS_AND_THEIR_SIMULANTS.

39 Bartelt-Hunt, S. L., Knappe, D. R. U. & Barlaz, M. A. A Review of Chemical Warfare Agent Simulants for the Study of Environmental Behavior. *Critical Reviews in Environmental Science and Technology* **38**, 112-136, doi:10.1080/10643380701643650 (2008).

40 Kongjan, P., Tohlang, N., Khaonuan, S., Cheirsilp, B. & Jariyaboon, R. Characterization of the integrated gas stripping-condensation process for organic solvent removal from model acetone-butanol-ethanol aqueous solution. *Biochemical Engineering Journal* **182**, 108437, doi:10.1016/j.bej.2022.108437 (2022).

41 Tang, X. *et al.* Adsorption and decomposition of dimethyl methylphosphonate on size-selected (MoO3)3 clusters. *Physical Chemistry Chemical Physics* **20**, 4840-4850, doi:10.1039/C7CP08427G (2018).

42 Kamalesh, R., Karishma, S., Saravanan, A. & Yaashikaa, P. R. Emerging breakthroughs in membrane filtration techniques and their application in agricultural wastewater treatment: Reusability aspects. *Sustainable Chemistry for the Environment* **8**, 100183, doi:10.1016/j.scenv.2024.100183 (2024).

43 Kim, Y. *et al.* Blocking chemical warfare agent simulants by graphene oxide/polymer multilayer membrane based on hydrogen bonding and size sieving effect. *Journal of Hazardous Materials* **427**, 127884, doi:10.1016/j.jhazmat.2021.127884 (2022).

44 Snider, V. G. & Hill, C. L. Functionalized reactive polymers for the removal of chemical warfare agents: A review. *Journal of Hazardous Materials* **442**, 130015, doi:10.1016/j.jhazmat.2022.130015 (2023).

45 Gorzkowska-Sobas, A. *et al.* Utilizing Zirconium MOF-functionalized Fiber Substrates Prepared by Molecular Layer Deposition for Toxic Gas Capture and Chemical Warfare Agent Degradation. *Glob Chall* **5**, 2100001, doi:10.1002/gch2.202100001 (2021).

46 Lee, J. *et al.* Mixed-matrix membrane reactors for the destruction of toxic chemicals. *Journal of Membrane Science* **605**, 118112, doi:10.1016/j.memsci.2020.118112 (2020).

47 Couzon, N. *et al.* Porous textile composites (PTCs) for the removal and the decomposition of chemical warfare agents (CWAs) – A review. *Coordination Chemistry Reviews* **467**, 214598, doi:10.1016/j.ccr.2022.214598 (2022).

48 Peng, C., Iqbal, Z., Sirkar, K. K. & Peterson, G. W. Graphene Oxide-Based Membrane as a Protective Barrier against Toxic Vapors and Gases. *ACS Applied Materials & Interfaces* **12**, 11094-11103, doi:10.1021/acsami.0c00615 (2020).

49 Song, Y. *et al.* Graphene Oxide and Metal–Organic Framework-Based Breathable Barrier Membranes for Toxic Vapors. *ACS Applied Materials & Interfaces* **14**, 31321-31331, doi:10.1021/acsami.2c07989 (2022).

50 Wang, W. *et al.* Machine learning assisted high-throughput computational screening of MOFs for the capture of chemical warfare agents from the air. *Separation and Purification Technology* **325**, 124546, doi:10.1016/j.seppur.2023.124546 (2023).

51 Li, A. *et al.* Machine learning-assisted development of gas separation membranes: A review. *Carbon Capture Science & Technology* **14**, 100374, doi:10.1016/j.ccst.2025.100374 (2025).

52 Sturluson, A. *et al.* The role of molecular modelling and simulation in the discovery and deployment of metal-organic frameworks for gas storage and separation. *Mol Simul* **45**, doi:10.1080/08927022.2019.1648809 (2019).

53 Mane, S., Dhote, R. R., Sinha, A. & Thirumalaiswamy, R. Digital twin in the chemical industry: A review. *Digital Twins and Applications* **1**, 118-130, doi:10.1049/dgt2.12019 (2024).

54 Giberna, M. *et al.* On Digital Twins in Defence: Overview and Applications. *Preprint at* https://arxiv.org/abs/2508.05717v1 (2025).

55 Ni, J. *et al.* Molecular fingerprint and machine learning enhance high-performance MOFs for mustard gas removal. *iScience* **27**, 110042, doi:10.1016/j.isci.2024.110042 (2024).

56 Yang, X. *et al.* Computational screening and machine learning of hydrophobic metal-organic frameworks for removal of chemical warfare agents from air. *Applied Materials Today* **31**, 101738, doi:10.1016/j.apmt.2023.101738 (2023).

57 Kianfar, E. A review of recent advances in carbon dioxide absorption–stripping by employing a gas–liquid hollow fiber polymeric membrane contactor. *Polymer Bulletin* **80**, 11469-11505, doi:10.1007/s00289-022-04626-z (2023).

58 Pedico, A., Baudino, L., Aixalà-Perelló, A. & Lamberti, A. Green Methods for the Fabrication of Graphene Oxide Membranes: From Graphite to Membranes. *Membranes (Basel)* **13**, doi:10.3390/membranes13040429 (2023).

59 Naidoo, M., Tai, S. L. & Harrison, S. T. L. Energy requirements for the in-situ recovery of biobutanol via gas stripping. *Biochemical Engineering Journal* **139**, 74-84, doi:10.1016/j.bej.2018.07.022 (2018).

60 Shao, G., Huang, X., Shen, X., Li, C. & Thomas, A. Metal–Organic Framework and Covalent–Organic Framework-Based Aerogels: Synthesis, Functionality, and Applications. *Advanced Science* **11**, 2409290, doi:https://doi.org/10.1002/advs.202409290 (2024).

61 Olawade, D. B. *et al.* Artificial Intelligence in Computational and Materials Chemistry: Prospects and Limitations. *Chemistry Africa* **8**, 2707-2721, doi:10.1007/s42250-025-01343-8 (2025).