EVALUATION OF THE ABILITY TO TRANSFORM YPERITE BY GREEN DECONTAMINATION BASED ON TUNGSTEN

Thanh Binh Vu[1,*], Ngoc Khue Do[1], Ngoc Toan Vu[1], Thanh Hoa Nguyen[2], Khanh Hung Nguyen[3], Duy Hung Dao[3]

[1]*Institute of New Technology, Academy of Military Science and Technology*
[2]*Thuyloi University*
[3]*Chemical Arms*

Abstract

This article presents the research findings on the evaluation of the ability to transform yperite (HD - a blister agent) of green decontamination based on tungsten. Several key factors influencing the decontaminating potential are thoroughly investigated, including the decontaminant-to-contaminant ratio, reaction temperature, and solution stability. Additionally, the decontamination efficiency on various materials such as paint, alumium, and L1 rubber fabric is also assessed. The results show that at a reaction volume ratio of 1:10, temperature ranging from 10ºC to 50ºC, and solution stability maintained for 18 hours, the decontamination efficiency on the aluminum surfaces exhibits the highest rate of 99.5%, followed by L1 fabric with 96.2% and paint with 77.8%; the density of decontaminant is recommended to apply 0.2-0.3 L/m^2. Moreover, the transformation mechanism of HD by the green decontamination agent is also proposed.

Keywords: *Yperite; green decontamination; tungsten.*

1. Introduction

Decontaminants represent substances or mixtures capable of converting contaminants into non-contaminant or less contaminating compounds. Previously, chlorine-based decontaminants such as hypochlorite, chloramine, and chloromelamine were widely utilized in the military context because of their high decontamination potential, low cost, and industrial availability. However, when exposed to organic agents containing aromatic rings, chlorine can form toxic dioxins, thereby posing long-lasting threats to both human beings and the environment [1]. Furthermore, the application of these compounds is also restricted because of their high corrosiveness, causing damage to equipments, weapons, and storage facilities. In recent decades, green chemistry (also known as clean chemistry, environmental chemistry, benign chemistry or sustainable chemistry) has emerged as a new development trend in both civilian and military domains. The environmental friendliness of chemical compounds is classified

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[*] Corresponding author, email: vuthanhbinh0979@gmail.com

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into three levels: edible, touchable, and usable [2], [3]. The ingredients of green decontamination (TDX-2) are environmentally friendly at different levels: Oxidant H_2O_2 3% used for wound cleaning, 1.5% used for mouthwash; K_2MoO_4 used in functional foods, vitamins; propylene glycol (PG) is a food additive; propylene carbonate (PC) is used as a solvent in cosmetics; the surfactant Triton X-100 (TX-100) is used in agriculture [2]. H_2O_2 is considered an ideal oxidant, exhibiting an atom economy of 47% with the sole byproduct of water. It is widely available in industry, and safe for storage, transportation and use. Nevertheless, the oxidative capacity of H_2O_2 alone often falls short in decontaminating highly toxic and poorly soluble substances, such as HD and VX. Therefore, study on catalysts for H_2O_2 has garnered noticeable attention from many researchers. Generally, H_2O_2 catalytic activators are classified into four groups, namely organic activators, metal ion activators, metal complexes (biomimetic), and metal salt activators. It is important to note that transition metal salt activators are of particular interest because of their uniqueness and robust catalytic potential. Tungsten compounds have been verified to be an ideal catalyst as they restrict the inefficient decomposition of H_2O_2 and are environmentally friendly [4]. In addition, a solvent system comprising of the surfactant TX-100, PC, and PG have also been proven to be promising thanks to their remarkable solubility for toxic agents, high adhesion and non-destructive effects on surface materials. Based on these findings, the composition of single components of TDX-2 has been developed and published, including H_2O_2 (3.09 M) as the oxidizer, K_2WO_4 (0.05 M) as the catalyst, K_2CO_3 (0.15 M) as a co-catalyst and alkalinity regulator, $K_3C_6H_5O_7$ (0.08 M) as a buffer and stabilizer, and the organic solvents TX-100, PC, and PG making up 40% of the volume [5]. This article evaluates the decontamination performance of TDX-2 in solutions and on various materials used for manufacturing military equipment. The study also identifies some transformation products and propose reaction mechanisms. While high-performance liquid chromatography (HPLC) is applied to quantify HD, gas chromatography-mass spectrometry (GC-MS) is employed to label the transformation products.

2. Experimental and research method

2.1. Reagents and apparatus

2.1.1. Reagents

HD was purified by distillation to a purity of 95%, H_2O_2 (30%) was obtained from Merck; TX-100 (99%); PC (99%); PG (99%); %); K_2WO_4 (99%), K_2CO_3 (99%), $K_3C_6H_5O_7$ (99%), Na_2CO_3 (99%) and Na_2SO_3 (99%) were purchased from Macklin; dichloromethane and methanol for HPLC were purchased from Fisher, single-distilled water.

2.1.2. Apparatus

High performance liquid chromatography agilent HP-1100 (USA) with a C8 column (250 mm × 4.6 mm × 5 µm), and UV-VIS diode array detector (DAD) with a scanning range of 0-1100 mm; gas chromatography-mass spectrometry (GC-MS), Agilent 5975 (USA) with a DB-5MS column (30 m × 0.32 mm × 0.25 mm); pioneer analytical electronic balance (Ohaus, USA) with a sensitivity of 0.0001 g; MS2 Minishaker (USA).

2.2. Research method

2.2.1. Research methods on the process of HD transformation in solution

The experiments investigating HD transformation using TDX-2 were conducted within 10 mL test tubes with lids as follows: Add 1 mL of TDX-2, followed by introducing of HD in proportions specified by the experimental design, after that, a vortex mixer was applied at a speed of 1800 rpm for 30 seconds to ensure homogeneity. At specific time intervals, a 59 µL sample was withdrawn and added to a test tube containing 1 mL of a reaction-stopping solution composed of 0.2 M Na_2SO_3 and 0.2 M Na_2CO_3 before being well-mixed. Subsequently, 2 mL of chloroform was then added, and the mixture was shaken for 2 minutes to extract the chloroform layer. This solution was then filtered via a 0.22 µm membrane filter and analysed using HPLC to identify the HD concentration [3]. All experiments were implemented in a fume hood under ambient pressure and room temperature.

2.2.2. Research methods on the HD decontamination efficiency on surface materials

The decontamination efficiency was assessed on three common materials surfaces, namely L1 protective rubberized fabric, military-grade green-painted wood, and uncoated metal (aluminum). The samples with smooth surfaces were thoroughly washed, drained and maintained under ambient temperature and humidity conditions. Each sample has an acreage of 10 cm × 10 cm and was bordered by a thin rim to prevent the solution from spilling over (wood samples were surrounded by a thin layer of paraffin, while the edges of aluminum and L1 fabric sampled were folded). Test material samples and decontamination agents were prepared as shown in Fig 1. Samples were contaminated with 90 µL HD equivalent to a density of 10 g/m^2, were then covered with a mica sheet to minimize excessive evaporation in the fume hood and left undisturbed for 1 hour. A certain of amount of newly made decontaminant TDX-2 was fairly distributed over the sample surfaces using a pipette before being evenly mixed for 1 minute and left untouched for 15 minutes under cover. After that, the excessive decontaminant was then discarded, and the samples were washed twice with 100 mL of distilled water each time.

The sheets were positioned upright, allowing them to dry naturally in the fume hood for 2 minutes. Once dried, the sheets were kept at 30°C, and the residual HD was extracted using 20 mL chloroform within 1 hour under cover. After 30 minutes, the process repeated similarly [2]. The two chloroform extracts were mixed afterwards and filtered with a 0.22 µm membrane filter, condensed to 1 mL with N_2 gas, which was then analysed using HPLC to identify the HD concentration after decontamination (C_t). A corresponding experiment without the decontamination process was conducted to establish the initial HD concentration (C_0). All experiments were implemented in a fume hood under ambient pressure and room temperature.

Decontamination performance (η, %) was measured using the following formula:

$$\eta = \frac{C_0 - C_t}{C_0} \cdot 100\,(\%) \tag{1}$$

where C_0 represents the initial HD concentration, C_t (ppm) represents the HD concentration after decontamination. Repeat each experiment 3 times, then take the average value. The experimental procedure is shown in Fig. 2.

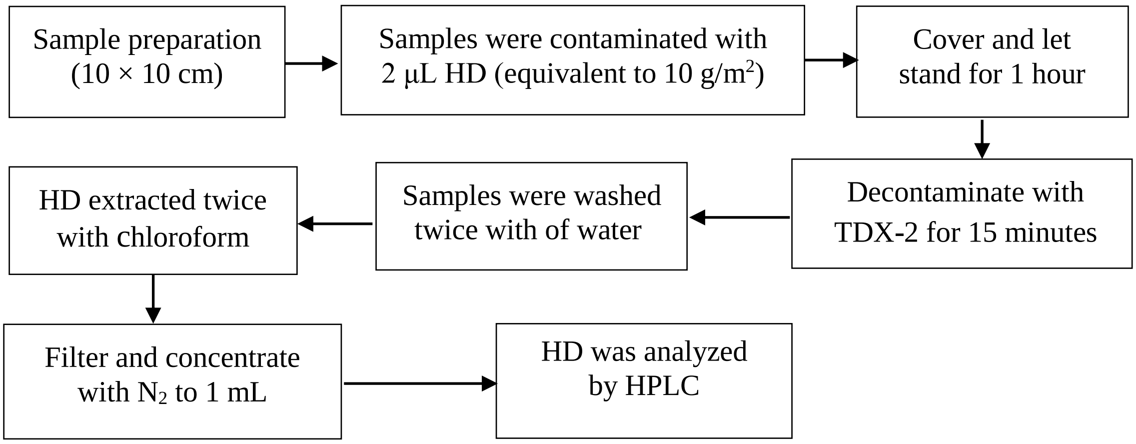


Fig. 1. General diagram of the testing process on the surface of materials.

Fig. 2. The experimental subjects for decontamination on the surface of the studied materials.

2.2.3. Research methods on quantifying HD using HPLC

The HD concentration at each designated time interval was analysed using the HPLC method with the following experimental conditions: Detection wavelength: 220 nm; Mobile phase: Methanol/water (V/V) = 70/30; Flow speed: 1 mL/minute; Injection volume: 10.0 µL; Retention time for the HD peak: $t_R = 4.816$ minutes.

2.2.4. Research methods on identifying transformation products using GC-MS

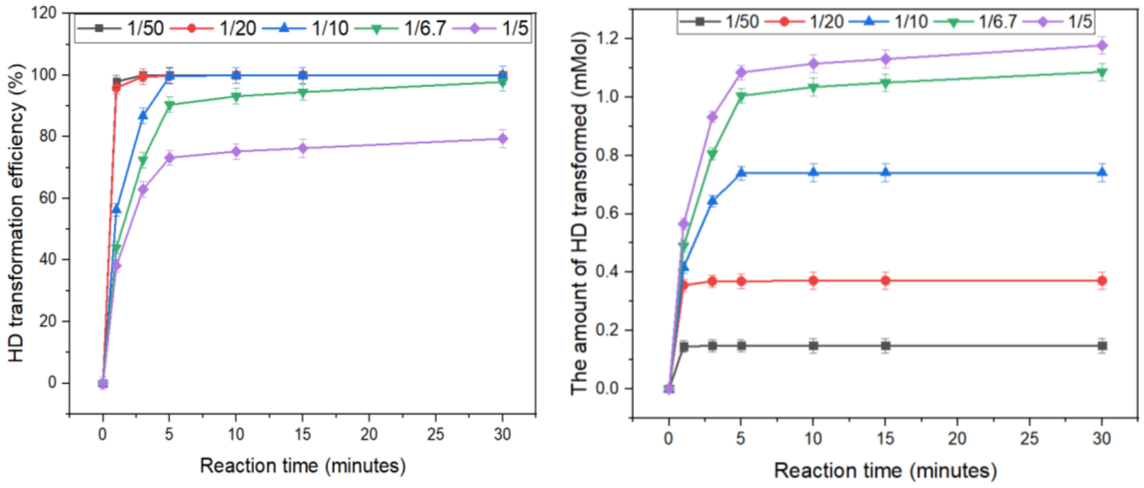
The chloroform extracts after being dried by using anhydrous Na_2SO_4 at a concentration of 0.1 g/mL were filtered via a 0.22 µm membrane filter and analysed through GC-MS to determine HD and other transformation products. The analytical conditions were as follows: Carrier gas: Helium; Initial temperature: 40^{o}C, held for one minute; Final temperature: 280^{o}C, held for 5 minutes; Heating rate: 10^{o}C/minute. Compounds were identified by comparing the mass spectra of the analytes with the NIST spectral library and using the fragment matching method.

3. Results and discussion

3.1. Evaluation of decontamination performance within solution

During use, the speed and transformation efficiency of decontaminants are the utmost pivotal factors to ensure the rapid and thorough treatment of toxic agents. The effectiveness of decontaminants can be enhanced by determining their maximum reactivity potential in a solution. This serves as a foundation for testing and evaluating their decontamination efficacy on various surface materials and under different conditions.

In assessing the decontamination performance of TDX-2 against HD contaminant in solution, reactions were conducted at the V_{HD}/V_{TDX-2} volume ratios of 1/50, 1/20, 1/10, 1/6.7, 1/5 (with the equivalent HD volume of 20 µL, 50 µL, 100 µL, 150 µL, 200 µL reacting with 1 mL of TDX-2). The experiments were implemented at 25^{o}C, following the procedures are illustrated in Section 2.2.1. On the outlook, at the ratio of 1/50, the reaction was mild with the solution being slightly warm; at the ratios from 1/20 to 1/15, the reaction was vigorous with the solution being increasingly hot and bubbly. After 5 minutes, almost all reactions ceased. At the ratios from 1/10 to 1/5, the solution appeared to be opalescent. The resulting evaluation of decontamination performance of TDX-2 is illustrated in Fig. 3.



(a) *(b)*

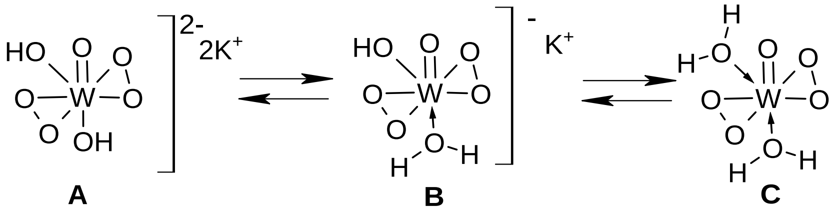
Fig. 3. (a) The effect of the ratio on HD transformation efficiency;
(b) The effect of the ratio on the amount of HD transformed.

As seen in Fig. 3, at the ratio from 1/50 to 1/10, the reaction proceeds rapidly with efficiency reaching 100% after 3 to 5 minutes with the amount of HD transformed corresponding to 0.148; 0.371, and 0.739 mmol. Meanwhile, at the ratios of 1/6.7 and 1/5, the reaction also happens quickly with efficiency achieving 73.21% and 90.38% after 5 minutes and the amount of HD transformed being 1.01 and 1.09 mmol; the efficiency then increases very slowly afterwards and ends with 97.83% and 79.39% efficiency after 30 minutes. These results indicate that the HD decontamination reactions by TDX-2 proceed swiftly, almost completing within 5 minutes. At the ratios from 1/50 to 1/10, HD was fully reacted, leaving the excess TDX-2. Additionally, at the ratios of 1/6.7 and 1/5, the reactions are almost complete after 5 minutes with the amount of HD converted around 1.01-1.09 mmol, at which point TDX-2 is entirely consumed. Therefore, with 1 mL of TDX-2, the reaction reaches its best at 1.01-1.09 mmol of HD in solution.

The above results can be explained as follows: In the aqueous phase, the catalytic precursor K_2WO_4 is rapidly oxidized by H_2O_2, forming the bisperoxotungstate complex [4], [6], [7]:

$$K_2WO_4 + 2\ H_2O_2 \rightarrow K_2[WO(O_2)_2(OH)_2] + H_2O \qquad (2)$$

The resulting bisperoxotungstate compound A is in equilibrium with B and C. The dianion in A is feebly active, while the mono- and di-protonated forms in B and C are sufficiently reactive [7].



(3)

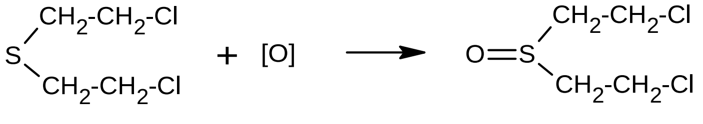
Bisperoxotungstate B and C made showcases high oxidative properties, the peroxo complex has strong oxidant properties approaches and oxidizes HD rapidly within 5 minutes, the subsequent reactions are predominantly hydrolysis.

Simultaneously, K_2CO_3 can be mixed with H_2O_2 to generate the peroxo complex HCO_4^-, which possesses significantly stronger oxidizing power than H_2O_2 alone [2], [8], [9]:

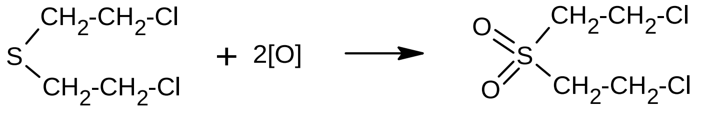
$$CO_3^{2-} + H_2O \leftrightarrow HCO_3^- + OH^- \quad (4)$$

$$HCO_3^- + H_2O_2 \leftrightarrow HCO_4^- + H_2O \quad (5)$$

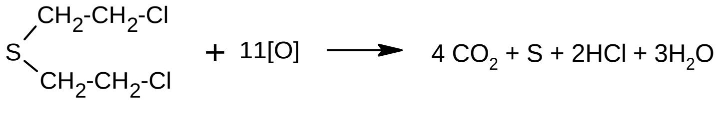
In 1 mL of TDX-2, the H_2O_2 concentration is 3.09 M, equivalent to 3.09 mmol. The amount of HD transformed, being 1.01-1.09 mmol, shows the maximum number of moles of HD equals to one-third of that of H_2O_2. This ratio aligns with the potential pathways for HD transformation at various levels, which may produce sulfoxide, sulfone, sulfide, or complete mineralization into CO_2, SO_4^{2-}, Cl^-, and H_2O. At the same time, a significant amount of heat generated during the reaction leads to the decomposition of a part of H_2O_2 and peroxo complex. The general reaction equations involved are as follows:



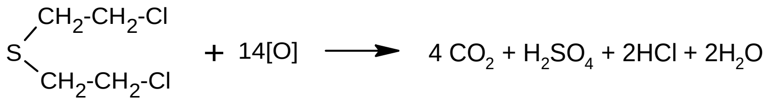
(6)



(7)



(8)



$$S(CH_2\text{-}CH_2\text{-}Cl)_2 + 14[O] \longrightarrow 4\,CO_2 + H_2SO_4 + 2HCl + 2H_2O \quad (9)$$

$$H_2O_2 \longrightarrow H_2O + O_2 \quad (10)$$

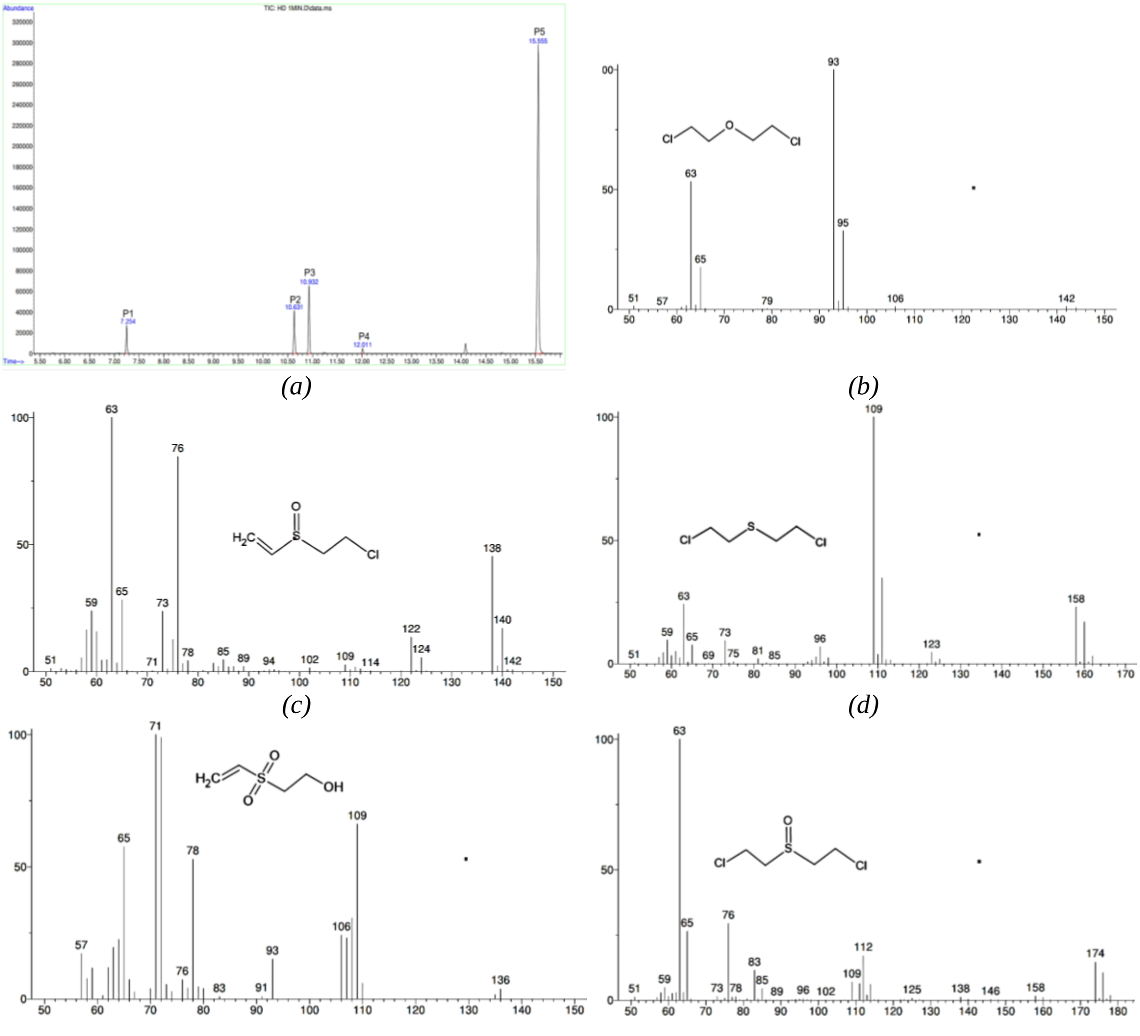
After 5 minutes of vigorous reaction, HD and other products continue to undergo hydrolysis in an alkaline environment.

3.2. Product identification and proposal of yperit transformation mechanism by TDX-2

As the toxic core of HD lies in the sulfur atom and the chloroalkyl group, the goal of decontamination processes is to oxidize the S atom to transform it into less toxic compounds, creating sulfoxide - a product with low level of toxicity and does not cause skin burns. At the same time, it is crucial to control excessive oxidation, leading to the formation of sulfone, which possesses high toxicity [10].

To determine the product formation tendency and propose transformation mechanisms, reactions are investigated at a reaction ratio of 1/10. Samples were analyzed using GC-MS as outlined in Section 2.2.4 at the reaction times of 0, 1, 10, and 30 minutes.

The GC chromatogram after 1 minute of reaction detects 5 peaks, including HD and other products with specific retention time of 7.254, 10.631, 10.932, 12.011, and 15.555 minutes, respectively. Based on characteristic ion fragments on MS spectra shown in Fig. 4, coupled with the comparison with the NIST library. The substances corresponding with these peaks are identified. In details, peak 1 is bis(2-chloroethyl) ether (with the m/z values of ion fragments of 63, 65, 93, and 95; match score of approximately 98%); peak 2 is 2-chloroethyl vinyl sulfoxide (with the m/z values of ion fragments of 63, 65, 76, and 138; match score of approximately 95%); peak 3 is bis(2-chloroethyl)sulfide (with the m/z values of ion fragments of 63, 109, 111, and 158; match score of approximately 97%); peak 4 is 2-hydroxyethyl vinyl sulfone (with the m/z values of ion fragments of 65, 71, 78, and 109; match score of approximately 96%); peak 5 is bis(2-chloroethyl)sulfoxide (with the m/z values of ion fragments of 63, 76, 112, and 174; match score of approximately 94%). Among these, peak 1 is identified as an inherent impurity, and peak 3 is the initial HD compound.



(a) *(b)*

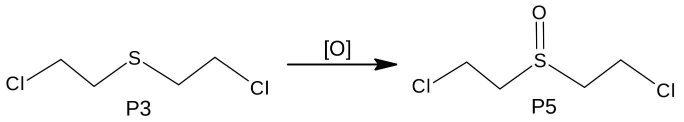
(c) *(d)*

(e) *(f)*

Fig. 4. (a) GC chromatogram of HD transformation products after 1 minute of reaction; (b) The MS spectrum of the product at t_R = 7.254 minutes; (c) The MS spectrum of the product at t_R = 10.631 minutes; (d) The MS spectrum of the product at t_R = 10.932 minutes; (e) The MS spectrum of the product at t_R = 12.011 minutes; (f) The MS spectrum of the product at t_R = 15.555 minutes.

The aliasing results in Fig. 5 show that, at the retention time of 10.932 minutes, the intensity of the corresponding HD of peak 3 decreases rapidly, with the reduction of 85% after one minute and peaks totally disappearing after 10 minutes. Therefore, HD can be considered to comprehensively transform, which consists of the experimental data presented in Section 3.1.

At the retention time of 15.555 minutes, the intensity of peak 5, relevant with bis(2-chloroethyl) sulfoxide, is high and relatively stable. From 1 minute to 10 minutes, during which HD is completely transformed, the peak undergoes subtle changes. Consequently, bis(2-chloroethyl) sulfoxide is regarded as the primary product of HD transformation using TDX-2. However, after 30 minutes, the intensity of the peak reduces to approximately 35%, indicating that it continues to transform into other products as follows:



(11)

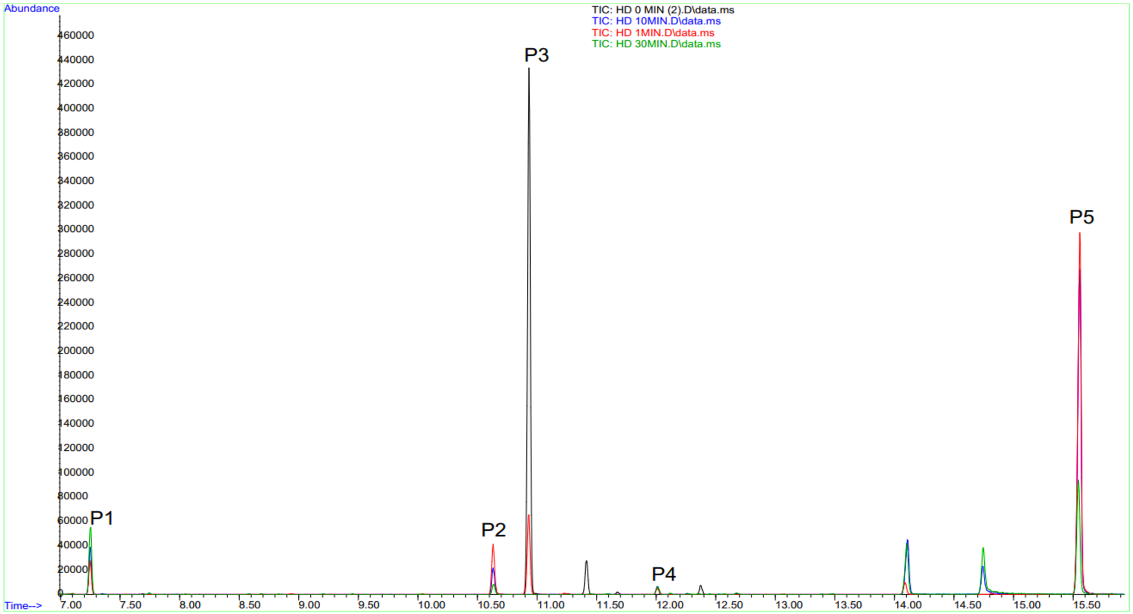
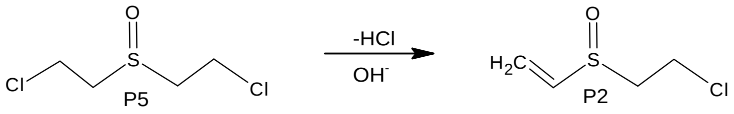


Fig. 5. The GC spectrum at reaction times 0, 1, 10, and 30 minutes (diluted 500 times).

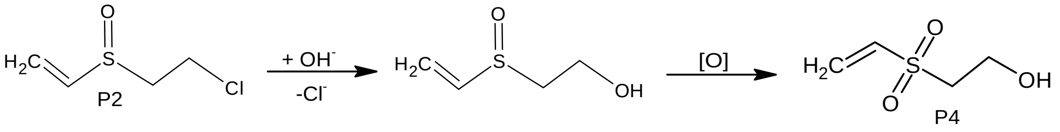
At the retention time of 10.631 minutes, the intensity of peak 2, relevant with 2-chloroethyl vinyl sulfoxide is not high and witnesses similar changes to peak 5, gradually reducing from 1 minute, 10 minutes, and further 30 minutes. This phenomenon can be explained that 2-chloroethyl vinyl sulfoxide is directly generated from bis(2-chloroethyl) sulfoxide in the alkaline environment and transformed into other subsequent products itself as follows:



(12)

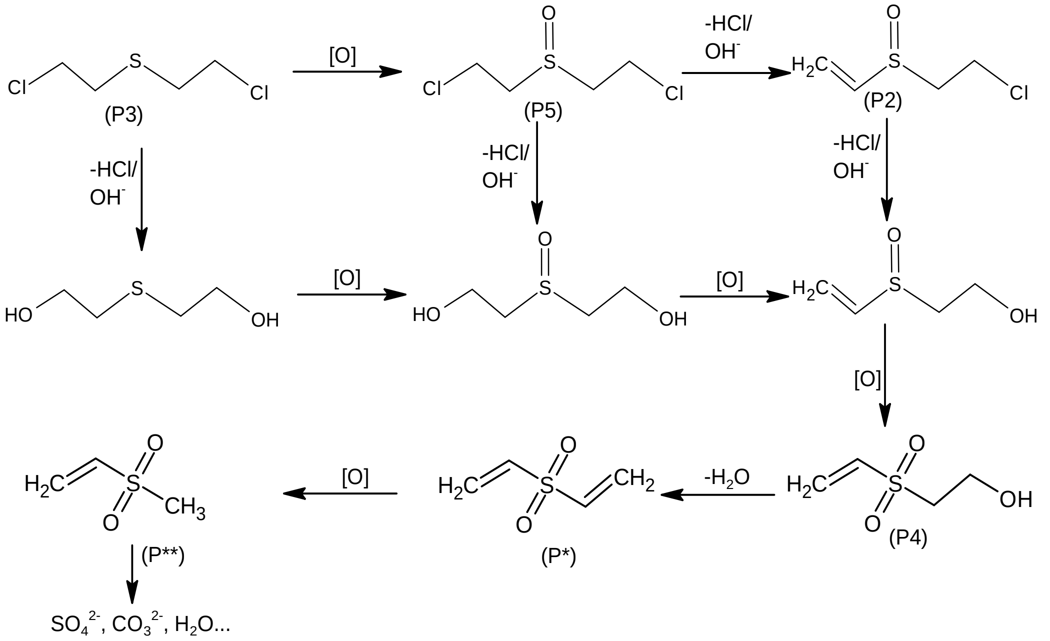
At the retention time of 12.011 minutes, the intensity of peak 4 is low and relatively stable. This phenomenon can be attributed to the good solubility of 2-hydroxyethyl vinyl sulfone in H_2O, making it more susceptible to hydrolysis than HD, resulting in its lower concentration in the chloroform extraction solvent [8].

Additionally, it may undergo further transformation into other products, and is even mineralized into CO_3^{2-}, SO_4^{2-}, H_2O as follows:



(13)

Based on the GC chromatographic analysis, the variation in peak intensities, and theoretical foundations, the mechanism of HD transformation by TDX-2 can be proposed as follows:



(14)

where P2, P3, P4, and P5 correspond to the peaks identified on the GC chromatogram at specific reaction time intervals. Products P* and P** also appear on the chromatogram at the retention times of 7.355 and 6.445 minutes, respectively, but with low intensities.

3.3. Decontamination efficiency depending on reaction temperatures

Considering climatic conditions in Vietnam, there is little difference between the ambient temperatures in hot and cold seasons. However, this remains an important factor affecting the decontamination efficiency of contaminated chemical warfare agents. To evaluate the impact of temperatures, three temperature points were investigated, 10°C, 25°C, and 50°C at the volume ratio of 1/10. The results are illustrated in Fig. 6.

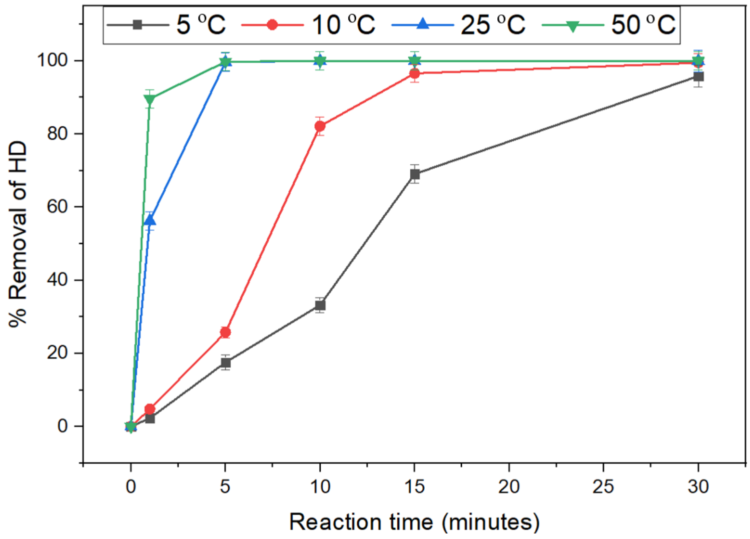


Fig. 6. The effectiveness of decontamination depends on the temperature.

As seen in Fig. 6, the higher the temperatures are, the faster reaction rate for the transformation of HD using TDX-2 is. At low temperatures, reaction efficiency depends more on temperature compared to reaction at higher temperatures. In the range from 25°C to 50°C, reactions happen rapidly and almost similarly, reaching the transformation efficiency of 100% with the mixture being scorching. At 5°C and 10°C, the reaction proceeds more mildly and slowly. At 5°C, reaction happens slowly during the first 10 minutes with the transformation efficiency achieving 33.22%, and accelerates afterwards, reaching efficiencies of 69.08% and 95.88% at 15 and 30 minutes, respectively. Meanwhile, at 10°C, the reaction is slow during the first 5 minutes, with a transformation efficiency of 25.80% and increases onwards, achieving 82.19% efficiency after 10 minutes and 96.6% after 15 minutes. These results align with the observed phenomena: at 5°C and 10°C, the initial mixture is cold, and the reaction proceeds slowly. As the reaction occurs, heat is released, causing the temperature to rise, accelerating the reaction. When the reactant quantities decrease, the heat release reduces, lowering the temperature and consequently slowing the reaction rate. These findings indicate that TDX-2 exhibits excellent decontamination performance for HD in the temperature range of 10-50°C at a reaction volume ratio of 1/10.

3.4. Evaluation of the stability of the solution

The decontamination process for contaminated chemical warfare agents requires the decontaminants being sprayed onto the affected surfaces. TDX-2 is maintained with 3 components which are well mixed before application. These days, modern equipment is already able to mix these components within a single device.

Nevertheless, under many circumstances, mixtures must be prepared hours prior to use. For that reason, in addition to speed and transformation efficiency, durability after preparation is also of paramount significance.

To investigate the durability of TDX-2, a study was conducted from 0 to 22 hours after mixing, stored at room temperature, with an HD/TDX-2 reaction volume ratio of 1/10. The results are presented in Fig. 7.

As seen in Fig. 7, HD decontamination reaction proceeds quickly with most of the HD being transformed after 5 minutes, aligning with the findings in Section 3.1. In addition, after 0 hour and 12 hours of mixing, the HD decontamination efficiency remains nearly equivalent, achieving 99% and 95% after 5 minutes of reaction and 100% after 10 minutes. As for TDX-2 stored for 18 hours, during which its efficiency declines, the efficiency is 97% after 10 minutes of reaction and 99.76% after 15 minutes. When stored for 22 hours, the decontamination rate decreases significantly, with the HD decontamination efficiency reaching 89.54% after 10 minutes of reaction and 96.27% after 30 minutes.

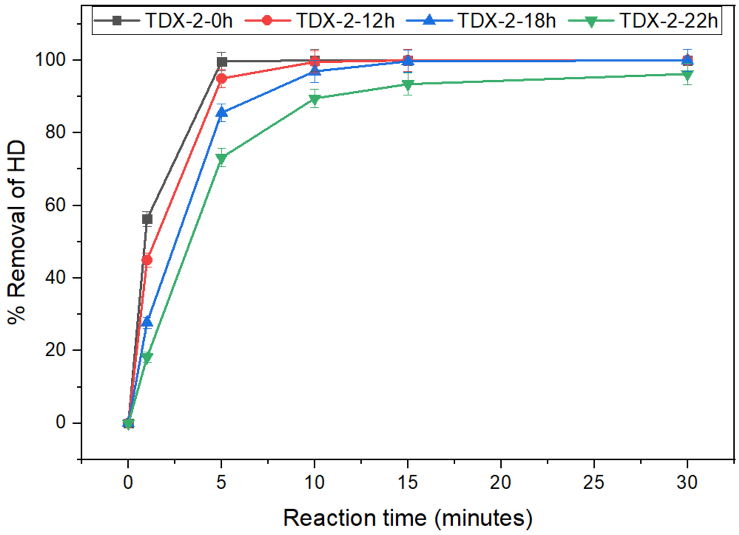


Fig. 7. The effect of solution mixing time on the decontamination rate of HD.

These results can be explained as follows: Because of the robust oxidative property of peroxide complexes, most of the HD contaminants are transformed after 5 minutes at the volume ratio of 1/10. In TDX-2, both bisperoxotungstate complex formed by K_2WO_4 and peroxo HCO_4^- formed by K_2CO_3 are simultaneously generated. While bisperoxotungstate with high stability though strong oxidative potential prevents unnecessary decomposition of H_2O_2 [4], peroxo HCO_4^- tends to decompose, releasing

O_2 and creating bubbles in solution, the higher the concentration of K_2CO_3 is, the less stable the solution becomes [2]. Therefore, the concentration of H_2O_2 decreases over time. The decontamination rate of TDX-2 stored for 18 hours significant declines after 10 minutes of reaction. This can be attributed to the depletion of H_2O_2 and the further hydrolysis of HD but at a much lower rate. According to the calculations in Section 3.1, the number of moles of H_2O_2 is approximately three times that of HD, indicating that after 18 hours, the remaining H_2O_2 of about 2.223 mmol is equivalent to 71.9%. It is also observed that the declining rate of H_2O_2 concentration accelerates over time, which requires further investigation.

3.5. Evaluation of decontamination potential on typical military materials

3.5.1. Evaluation of decontamination efficiency on various materials

While decontaminating warfare toxins adhered to the surface of weapons, the ability of the detoxifying solution to penetrate the material surface significantly influences the amount of solution required and the overall treatment efficiency. Military facilities in general, and chemical equipment in particular, typically contain three types of surfaces: A – painted surfaces (including both metals and wood), B – unpainted metal surfaces (aluminum, steel…), and C – L1 fabric surfaces (used in L1 chemical protective clothing) as seen in Fig. 8.

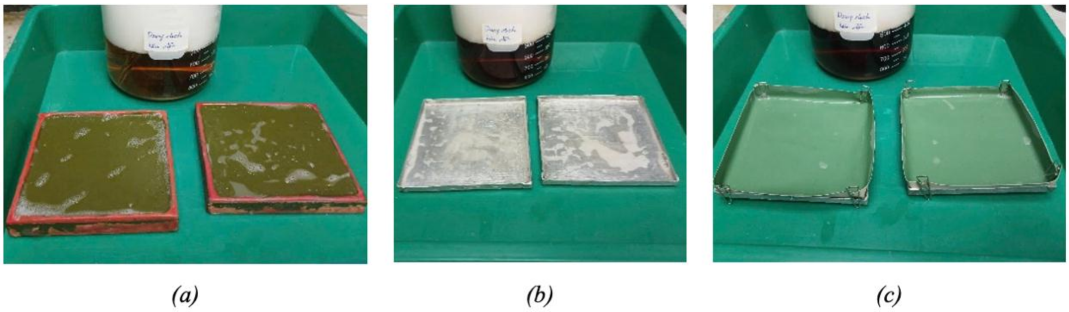

(a) (b) (c)

Fig. 8. Determination of decontamination efficiency on various surface materials.

The evaluation of HD decontamination efficiency using TDX-2 on the surfaces of various materials is conducted as follows: the HD concentration is 10 g/m^2, the application concentration of the decontaminants is 0.5 L/m^2, following the procedures outlined in Section 2.2.2 and comparing the findings with the decontaminant TDX-1 [11] and several US agents previously reported, including Decon Green (DG), New Decon Green (NDG), and DF-200 [2]. TDX-2 and TDX-1 were mixed 30 minutes before use. The results are presented in Tab. 1.

Tab. 1. Decontamination efficiency of HD on various surface materials

Subjects	**Time(min)**	**TDX-2**	**TDX-1**	**DG**	**NDG**	**DF-200**
A	10	77.8	78.2	-	-	-
	15	80.2	80.5	92.2(*)	79.0(*)	62.9(*)
B	10	99.0	99.3	-	-	-
	15	99.5	100	99.91	99.90	-
C	10	95.0	95.8	-	-	-
	15	96.2	97.0	-	-	-

* *Testing on CARC (Chemical Agent Resistant Coating) paint surface* [2].

From Tab. 1, it can be observed that the decontamination efficiencies of TDX-2, TDX-1, and NDG are comparable, DG seems to have higher efficiency while that of DF-200 is lower. These results can be attributed to the variations in solvent system, oxidizing agents, and catalysts. A large amount of organic solvents, including 60% VPC and 10% VTX-100, in DG enables it to dissolve highly viscous toxins like HD and VX more effectively though it can damage the paint and fog the mask lenses. TDX-2, TDX-1, and NDG possess the same solvent systems, including 20% VPC, 10% VPG, 10% VTX-100, which develop from DG, causing little damage to material surfaces while still ensuring the good dissolution of toxins [2], [8]. Meanwhile, DF-200 with approximately 1-4% cationic surfactants weakens the ability to dissolve toxins. Considering the oxidant systems and catalysts, DG, NDG, and TDX-1 all use the H_2O_2/K_2MoO_4 system with relatively similar concentration. TDX-2 with the H_2O_2/K_2MoO_4 system of lower concentration tends to be more stable while delivering equivalent effectiveness. Noticeable, DF-200, as an older version, with the $H_2O_2/KHCO_3$ system of low concentration brings about lower effectiveness.

In comparison with the decontamination efficiencies between various surfaces, it can be obeserved that aluminum surface achieves the highest efficiency while that of painted surface is the lowest. These results are because of the HD permeability of the materials. As the contaminant can not penetrate aluminum surface, it can easily be decontaminated. Whereas the painted and L1 surfaces absorb a certain amount of HD, reducing the decontamination efficiency compared to aluminum. L1 fabric, which is a specialized rubber material used for chemical protective clothing, absorbs less HD than painted surfaces, resulting in better decontamination efficiency compared to the painted surfaces.

3.5.2. Evaluation of the density of decontamination

In the process of decontamination, the decontamination density represents the amount of decontaminants needed for treating toxins to a safe level over a unit area. This is an exceptionally pivotal parameter ensuring the efficient, safe, and cost-saving usage of decontaminants. In pursuit of decontamination density evaluation, experiments are conducted following the procedures outlined in Section 2.2.2. on the surfaces of 3 material subjects described in Section 3.5.1 with the density of 0.1, 0.2, 0.3, 0.4, and 0.5 L/m^2. From visual assessment, at the density from 0.2 L/m^2 to 0.5 L/m^2, the decontaminants fully cover the surfaces, while they only cover partially the subject surfaces at the density of 0.1 L/m^2. The results are presented in Tab. 2.

Tab. 2. The effect of decontamination density on decontamination efficiency

Subjects	**Density (L/m^2)**				
	0.1	**0.2**	**0.3**	**0.4**	**0.5**
A	75.8	83.8	84.1	84.2	84.6
B	96.5	98.2	99.3	99.5	99.5
C	90.6	95.5	96.0	96.0	96.2

From Tab. 2, it can be generally observed that there is an increase in the decontaminant efficiency as a result of the rise in its density for all three subjects. This finding is comprehensively consistent with the results shown in Section 3.1 since higher density helps to strengthen the ability to dissolve toxic agents and increases reaction rate. Moreover, at the density from 0.2 L/m^2 to 0.5 L/m^2, the efficiency is comparable, whereas the decontamination efficiency witnesses a significant decrease at the density of 0.1 L/m^2. These results can be attributed to the fact that, with the toxic agents distributed on the subject surfaces at the density of 10 g/m^2, the contaminants form into small droplets instead of covering the surfaces evenly. Consequently, at very low decontaminant densities, the reaction rate within these droplets cannot be ensured, and in some areas, the decontaminant is insufficient to provide complete coverage. Based on the above findings, the decontamination density is proposed to be in the range of 0.2-0.3 L/m^2 at the HD contamination density of 10 g/m^2.

4. Conclusion

The yperite transformation pathways in solution and on various surfaces of military equipment by TDX-2 based on tungsten have been studied. The research results indicate that TDX-2 exhibits effective decontamination of HD. In solution, the decontamination reaction achieves high efficiency at a ratio of 1/10 and temperatures ranging from 10°C to 50°C, with a tendency to produce sulfoxide, which is non-caustic to the skin. In addition, TDX-2 represents a decontaminant with high stability, and decontamination efficiency being well-maintained for 18 hours after mixed. On the material surfaces, the decontamination efficiency depends on the permeability of the materials. Aluminum surfaces achieve the best decontamination efficiency, followed by L1 fabric and painted surfaces with the recommended decontamination density for these surfaces ranging between 0.2 and 0.3 L/m².

References

[1] V. T. Bình và nnk, *Chất tiêu tẩy và phương pháp tiêu tẩy*, Hà Nội: Nxb Quân đội Nhân dân, 2017.

[2] G. W. Wagner *et al.*, "Development of new decon green: A how-to guide for the rapid decontamination of CARC paint", US Army Research, Development and Engineering Command, 2008.

[3] G. W. Wagner, "Hydrogen peroxide-based decontamination of chemical warfare agents", *Main Group Chemistry*, Vol. 9, No. 3-4, pp. 257-263, 2010. DOI: 10.3233/MGC-2010-0028

[4] R. Noyori *et al.*, "Green oxidation with aqueous hydrogen peroxide", *Chemical Communications*, No. 16, pp. 1977-1986, 2003. DOI: 10.1039/B303160H

[5] V. T. Bình và nnk, "Nghiên cứu xây dựng thành phần đơn và đánh giá quá trình chuyển hóa 2-chloroethyl phenylsulfide của chất tiêu độc xanh trên cơ sở vonfram" *Tạp chí Nghiên cứu Khoa học và Công nghệ quân sự*, Số 94, tr. 109-116, 2024. DOI: 10.54939/1859-1043.j.mst.94.2024.109-116.

[6] N. T. Thủy và nnk, "Xúc tác trên cơ sở kim loại trong phản ứng epoxy hoá dầu đậu nành", *Tạp chí Hóa học*, Tập 53, Số 4, tr. 515-519, 2015. DOI: 10.15625/0866-7144.2015-00172

[7] N. T. Thủy và nnk, "Ảnh hưởng của các thành phần trong hệ xúc tác Wonfram đến phản ứng Epoxy hoá dầu đậu nành", *Tạp chí Khoa học Đại học quốc gia Hà Nội: Khoa học Tự nhiên và Công nghệ*, Tập 33, Số 1, tr. 81-87, 2017. Available: https://js.vnu.edu.vn/NST/article/view/4194 [Accessed Dec. 10, 2024].

[8] G. W. Wagner *et al.*, "Decon Green: The environmentally-friendly decontaminant", 3th Singapore International Symposium on Protection Against Toxic Substances, 2002.

[9] M. Kassem *et al.*, "Oxidative decontamination of sulfur mustard using formulations based on hydrogen peroxide", The International Conference on Chemical and Environmental Engineering, Military Technical College, 2008. DOI: 10.21608/iccee.2008.38421

[10] G. W. Wagner *et al.*, "Molybdate/Peroxide oxidation of mustard in microemulsions", *Langmuir,* Vol. 17, No. 16, pp. 4809-4811, 2001. DOI: 10.1021/la010334h

[11] T. B. Vu *et al.*, "Research on formulating ingredients and evaluating the decomposition ability of 2-chloroethyl phenylsulfide by green decontamination based on molybdate", *Journal of Military Science Technology,* Vol. 90, pp. 94-101, 2023. DOI: 10.54939/1859-1043.j.mst.90.2023.94-101

ĐÁNH GIÁ KHẢ NĂNG CHUYỂN HÓA YPERITE BỞI DUNG DỊCH TIÊU ĐỘC XANH TRÊN CƠ SỞ VONFRAM

Vũ Thanh Bình[1], Đỗ Ngọc Khuê[1], Vũ Ngọc Toán[1], Nguyễn Thanh Hoà[2],
Nguyễn Khánh Hưng[3], Đào Duy Hưng[3]

[1]*Viện Công nghệ mới, Viện Khoa học và Công nghệ quân sự*

[2]*Đại học Thuỷ Lợi*

[3]*Binh chủng Hoá học*

Tóm tắt: Bài báo trình bày kết quả nghiên cứu đánh giá khả năng chuyển hóa yperite (HD - chất độc loét da) của chất tiêu độc xanh trên cơ sở tungsten. Một số yếu tố chính ảnh hưởng đến khả năng tiêu độc đã được khảo sát, gồm: Tỉ lệ phản ứng giữa chất độc và chất tiêu độc, nhiệt độ phản ứng, độ ổn định của dung dịch. Đồng thời hiệu quả tiêu độc trên một số loại vật liệu đã được thử nghiệm như: sơn, nhôm, vải cao su L1. Kết quả cho thấy, ở tỉ lệ 1/10 về thể tích, nhiệt độ từ 10°C đến 50°C, dung dịch ổn định trong 18 giờ và hiệu quả tiêu độc trên bề mặt nhôm đạt cao nhất 99,5%, sau đó đến vải L1 96,2% và sơn 77,8%; mật độ chất tiêu độc được đề xuất sử dụng từ 0,2 L/m^2 đến 0,3 L/m^2. Đồng thời cơ chế chuyển hóa HD bởi chất tiêu độc xanh đã được đề xuất.

Từ khóa: *Yperite; tiêu độc xanh; tungsten.*

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