Al-Hetty *et al. BMC Chemistry* (2025) 19:120
https://doi.org/10.1186/s13065-025-01495-1

BMC Chemistry

RESEARCH Open Access

Numerical simulation of stability of diffusion depth of deterrents into cylindrical nitrocellulose composite under different conditions

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Abstract
In this study, evaluation and prediction of diffusion depth of deterrents of Butyl-NENA and Polyethylene-glycol-di-methacrylate into the propellant and the effect of different conditions on diffusion stability, such as variations of concentration, temperature and aging with time, were performed by using COMSOL Multi-physics 4.4 to lower the laboratory costs and saving time. Diagrams indicated that diffusion of deterrents occurs to a certain depth of the propellant radius and variations of concentration in allowed ranges, does not affect the final diffusion depth significantly. Also, variations in temperature and aging with time had a little effect on the diffusion depth. Results showed that substances were used for nitrocellulose propellant coating, have excellent diffusion stability. simulation results were compared torelated experimental results and showed good agreement with them. concentration profiles of Butyl-Nena at two concentrations of 10% and 20%, measured at 70˚C for 10 h. the concentration profile at 10% is shown, and a gentle increase in concentration is observed for small to medium radii. While the 20% profile shows a faster and more significant increase in concentration, reaching high values at larger radii. These results indicate a significant effect of Butyl-Nena concentration on its concentration distribution pattern with increasing radius. the concentration profiles of deterrent polymers at two concentrations of 2% and 12%, measured at 70˚C for 10 h. the deterrent concentration at 2% gradually increases and reaches significant values, while at 12%, the concentration rapidly approaches a maximum value. These results indicate a significant effect of deterrent concentration on the concentration profiles with increasing radius.The aim of the present work was predicting the influence of various conditions such as, concentration, temperature and time on deterrents diffusion stability by COMSOL Multi-physics.

Keywords Nitrocellulose, Deterrent, Simulation, COMSOL Multi-physics, Diffusion, Stability

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Introduction

Nitrocellulose (NC), a kind of energetic material, has been widely used in the industrial and military fields for celluloid, photographic plate, glasses frame, lacquers, paints, solid rocket propellants and explosives [1–6]. As the self-reactive chemical substance, NC generally undergoes a sharp exothermic runaway reaction at elevated, even normal temperatures owning to the characteristic of high energy material [7–10]. Its unique hazardous properties, such as high impact sensitivity, poor chemical stability, flammability and explosive hazards, are greatly dangerous during the storage process [11–15]. Not long ago, nitrocellulose attracted people's attention since a particularly significant fire explosive disaster occurred at Tianjin port in China, which caused 165 people deaths, 8 missing people and 798 injuries [11]. The direct cause of the accident was the loss of the humectants, which resulted in local desiccation and heat accumulation on account of exposure to the sun in summer for long periods and the poor heat dissipation in the containers. Therefore, it is extraordinary to carry out relevant in-depth researches on the influencing factors during storage [16–20].

Nitrocellulose propellants are coated with substances called deterrent to prevent them from unwanted combustion to contact with oxygen during shelf life and reduce their burning rate when they are launched and in quick contact with oxygen to avoid them not to burn earlier than the desired time. It should be considered to choose deterrents that penetrate to a certain depth in the propellant and do not diffuse deeper with time, change in temperature or change in concentration of deterrents [21–25]. Therefore, the stability of diffusion depth of deterrents that are diffused in the propellant is very important and necessary. Deterrents are divided into two categories of small molecules and polymers. Desired chemical and mechanical properties could not be enhanced by one deterrent, so several types of it, usually are used for coating [1, 26–27].

Using computational fluid dynamics (CFD) to simulate fluid issues, has been increased significantly in the last thirty years and has made different branches of science and engineering more disciplined.Recent advances in CFD coding, have enabled researchers to make simply graphical images of speed, temperature, soluble component concentration and pressure fields in the domain [4]. CFD simulation is a powerful tool that is applicable for simulating industrial and non-industrial phenomena [5, 6]. Propellant performance can be improved by knowing deterrents penetration rate. Another important parameter is the deterrents penetration rate during aging and propellant shelf time that is called migration, because it affects its life time. Migration calculation is often difficult, expensive and time consuming, so progressing simulation tools of these processes is important. Folly et al. simulated migration of both nitroglycerin and deterrents within swollen nitrocellulose matrix with AKTS-SML software. Furthermore, after determining the temperature dependence on diffusion coefficient, it was possible to determine deterrents migration in different temperature profiles. This study showed some benefits of simulating oil and deterrent diffusion into nitrocellulose propellant [7].

A three-layer system was introduced by Levy that studied some types of spherical propellants by light microscopy and was used to analyze simulation results of Foley et al.'s work [8].

Their simulation results showed a good agreement with experimental observations that higher rate of oil penetration to the propellant matrix occurs in presence of deterrent. Simulations showed that oil penetrates faster in zones containing deterrent than the zones with zero deterrent concentration. Comparison of simulated migration and experimental curves showed good agreement between them. Results indicatedthat the smallest changes in temperature, even after a short period of time can cause a shift in deterrent concentration profiles [9, 17–23]. Several works have been done on diffusion phenomena with COMSOL Multi-physics software, but so far, simulation of deterrents diffusion into nitrocellulose propellant has not been done with it. Due to the software capabilities and saving the costs of producing and testing samples, it was used for this work. The aim of the present work was predicting the influence of various conditions such as, concentration, temperature and time on deterrents diffusion stability by COMSOL Multi-physics.

Experimental

Materials

A double-based nitrocellulose propellant containing:

- 87% of nitrocellulose, as the basic propellant.
- 10% of 2-Nitroxy-Ethyl-Nitramine plasticizerabbreviated to Buthyl-NENA.
- 2% of the deterrent of Polyethylene-Glycol-Dimethacrylate with themonomer of 3-Ethylene-Glycol-Dimethacrylate.
- 1% of stabilizersandotheradditives.

Preparation method

A cylindrical nitrocellulose propellant was made with a length of 2.98 mm and a diameter of 1.79 mm. 7 small bores with a diameter of 0.12 mm were shaped as one in the center of the propellant and 6 apart of the center with equal distance of 0.36 mm. Propellants were washed with distilled water before coating to be purified from impurities. Then plasticizer was added and timed. After that, deterrent monomers were added and polymerization was done on the propellant surface in certain conditions [3]. The present work was done in order to lower the cost of performing changes in real reactors and avoid the probable damages.

Theory

Diffusion during deterrentation can be occurred by Fickian or non Fickian (case Ⅱ) mechanism. No information about the mechanism of diffusion during the shelf time is available. The equation for one-dimensional diffusion profiles in heterogenous domain is:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{1}$$

C is the concentrationof diffusive deterrent [g/m^3], t is the diffusion time [s], D is the diffusioncoefficient[m^2/s] and x is the distance [m]. This equation can be used for changes of boundary conditions provided that thediffusion coefficient remains constant:

$$c(x,t) = \frac{S}{\sqrt{\pi\,D\,t}}e^{\frac{-x^2}{4\,D\,t}} \tag{2}$$

Equation (2) Describes immediate start of diffusion in the surface. S is the deterrent concentration at surface[g/m^2] [10].

Simulation

The limitations of these equations during simulation are:

- The diffusion process has to occur in monolayer structures following the Fick's laws.
- The diffusion coefficient must be constant during the experiment.
- No other phenomena contribute the mass transfer e.g., evaporation on the surface or chemical reactions between matrix and diffused molecules or between different migrating compounds [9].

No moving boundary was considered for polymeric deterrent because large molecules cause no inflation in the matrix; the inflation caused by small molecule of plasticizer can be neglected. There is no drying in the first stage of coating and the created layer on the propellant can be considered as infinite solution. The temperature influence was applied by the diffusion coefficient. The penetration was carried out from the surface to the inside of the matrix in the radius direction with no exit and extremelylowrate. The bores that were installed to better drying the propellant after coating, soplotting themin the propellant geometry was ignored since the diffusion of the solution in these regions was negligible [11–13]. For better results, it was considered that two materials with different diffusion coefficients, penetrate into the solid matrix of nitrocellulose from an infinite solution. The parameters required for simulation are given in Table 1.

Table 1 The parameters required for simulation [3, 9, 14]

Name	Expression	Description
R1	895 [micrometer]	NC matrix radius
H	2.98 [*mm*]	Length
M_B	150 [*g/mole*]	Molecular weight of Butyl-NENA
b1	0.1*m	Inlet weight of Butyl-NENA
C_B_max	b/(M_B*V)	Inlet concentration of Butyl-NENA
a	1000	Dimensionless factor
M_D	11,000 [*g/mole*]	Average molar mass of polymeric deterrent
M_monomer	286.3 [*g/mole*]	Molar mass of monomeric deterrent
D_D	1.64e-17 [*m^2/s*]	Diffusion coefficient of deterrent
b2	0.02*m	Inlet mass percent of deterrent
C_D_max	b2/(M_monomer*V)	Inlet concentration of deterrent
D_B	1.14e-16 [*m^2/s*]	Diffusion coefficient of plasticizer in double_ base propellant

Table 2 Temperature dependent diffusion coefficient [14]

Temp (˚C)	D_B [m^2/s]	D_D [m^2/s]
40	1.14e-16	1.64e-17
50	4.6e-16	6.56e-17
60	1.84e-15	2.62e-16
70	7.35e-15	1.05e-15

Concentration variations of the plasticizer from 10 to 20% and the polymeric deterrent from 2 to 10% with an increase of 2% in each stage, at 40, 50, 60 and 70 ° *C* for 4 h were applied to cover the required temperature and time ranges. Considering that each 10 degree increase in temperature, increases 4 times the diffusion coefficient of the particles, so temperature variations were applied to change the diffusion coefficients which is given in Table 2 and the effect of temperature on the diffusion was studied separately with concentration variations. Therefore, the average of diffusion coefficients was obtained according to the particle molecular weight that was mentioned in [9, 14]. A two-dimensional symmetric meshview, is shown in Fig. 1.

Results and discussion

Effect of temperature

Figure 2 shows the concentration profiles of butyl Nena in terms of nitrocellulose radius at 40, 50, 60 and 70 °C inthe presence of the polymer for 4 h. It is seen that with increasing the temperature, the particles penetrate more deeply. Precisely, the particles diffuse to the depth

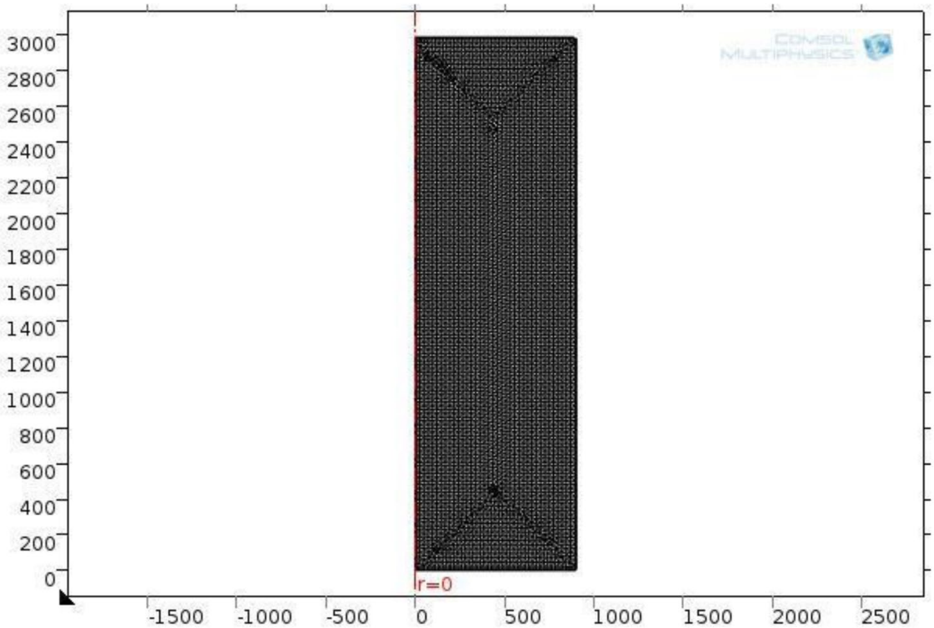

Fig. 1 A meshviewgenerated in two-dimensionalmodel

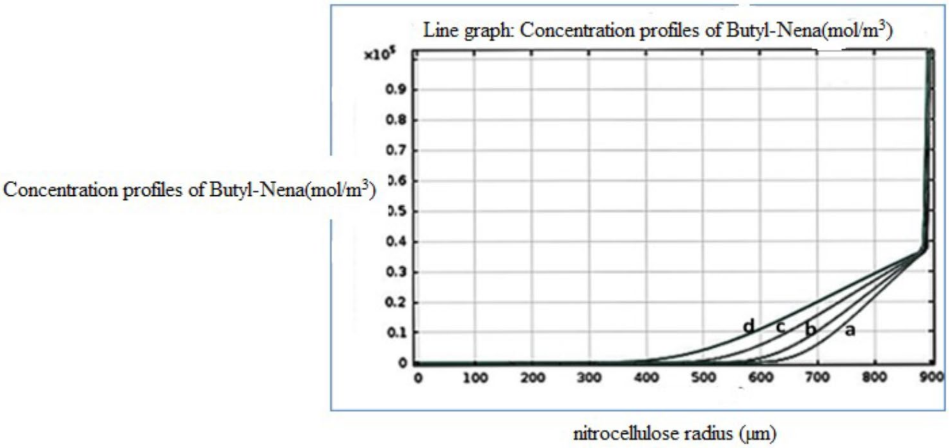

Fig. 2 Concentration profiles of 10% Butyl-Nena interms of nitrocellulose radius in different temperaturesfor 4 h. (a) 40 ° C, (b) 50 ° C, (c) 60 ° C, (d) 70 ° C

of 600 micrometers at 40 °C. the molecules penetrate to 550 micrometers at 50 °C. Penetration occurs to 450 micrometers at 60 ° C and at the highest temperature of 70 ° C, Butyl Nena molecules penetrate to the depth of 400 micrometers. But, it is seen that at all temperatures, nearly 60% of Butyl-Nena particles penetrate to the depth of 890 micrometers so they remain near the surface. The variations between the diagram slopes indicates that the amount of particles in deeper radius goes higher by increase in temperature.

Figure 3 shows the concentration profiles of polymeric deterrent in terms of nitrocellulose radius at 40, 50, 60 and 70 ° C inthe presence of Butyl-Nena for 4 h. It is seen that with increasing temperature, the molecules penetrate more deeply, but changes in diffusion depth are lower than those for butyl-Nena.More specifically, in four stages of change in temperature, the diffusion depth of the polymerchanges within the radius of 500 to 400 micrometers.It is seen that at all temperatures, nearly 70% of the polymer particles penetrate to the depth of 890 micrometers so they remain near the surface. Like the profiles of Fig. 2, the variations between the diagram slopes indicates that the amount of particles in deeper radius goes higher by increase in temperature, but change in diagram slopes of polymeric deterrent is lower than Butyl-Nena profiles. This means that change in temperature affects on diffusion depth of butyl-Nena more than that of the polymer. Based on references, the greater penetration of polymer rather than Butyl-Nena at 40 ° C could be due to the reason that Butyl-Nena, which has

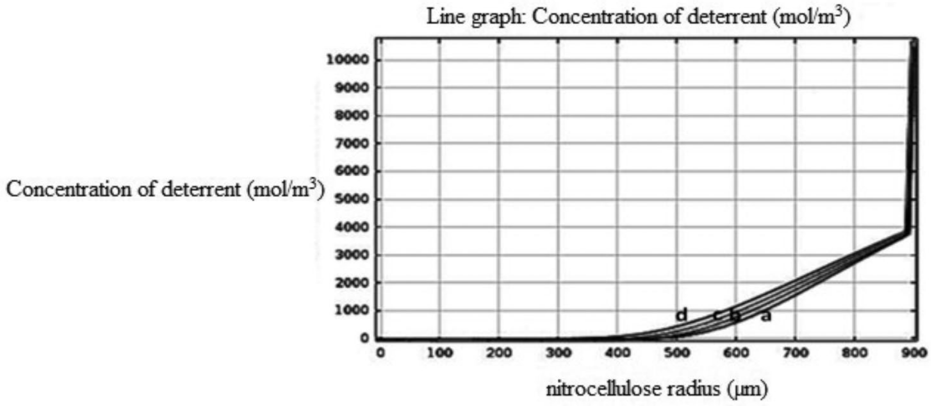

Fig. 3 Concentration profiles of 2% polymeric deterrent interms ofnitrocellulose radius in different temperaturesfor 4 h. (a) 40 ° C, (b) 50 ° C, (c) 60 ° C, (d) 70 ° C

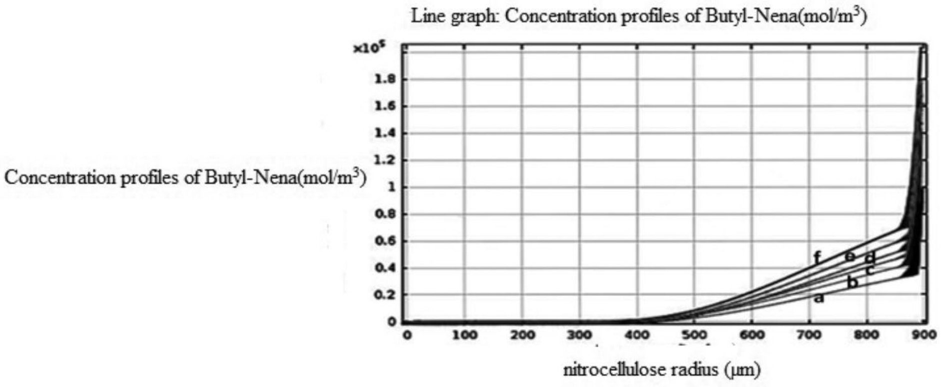

Fig. 4 Concentration profiles of 10–20% Butyl-Nena in terms of nitrocellulose radius at 70˚C for 4 h. (a) 10% Butyl-Nena, (b) 12% Butyl-Nena, (c) 14% Butyl-Nena, (d) 16% Butyl-Nena, (e) 18% Butyl-Nena, (f) 20% Butyl-Nena

small molecules acts as a plasticizer for the polymer and causes more penetration in nitrocellulose at this temperature [9].

Effect of concentration

Figures 4 and 5 show the concentration profiles of 10–20% Butyl-Nena and 2–12% polymeric deterrent in terms of nitrocellulose radius at 70 ˚C for 4 h, it can be found that variations in concentration of both substances at 70 ° C only affect the slope of diagrams and increase the particles concentration in the middle, but at this temperature, the penetration depth of a few micrometers may not change the final diffusion depth. In the surface, the concentration amount of both plasticizer and polymeric deterrent is the highest and is reduced to the middle part sharply and becomes near to zero to the depth of 400 µm and remains zero from 400 µm to the center. No considerable shift in diffusion depth is caused by 10 to 20% change in Butyl-Nena concentration and 2 to 12% change in polymeric deterrent concentration, becausethe temperature is constantand the particles diffusion coefficient is temperature dependent [14–16], but since the concentration increases, the amount of particles that penetrate deeper becomes higher and the slopes of the diagrams grow further.Option of 70 ° C was to see the highest variations.

Effect of time on diffusion stability

The effect of time on diffusion stability in the amount of 10 and 20% of plasticizer and 2 and 10% of polymeric deterrent at 70˚C after 10 h was studied. Comparison of Figs. 6 and 7 with the former diagrams which the considered time was 4 h, revealed that the variations occur in the same regions of the propellant radius for both substances and the ultimate penetration depth does not change substantially. Figure 6 shows the concentration profiles of Butyl-Nena at two concentrations of 10% and 20%, measured at 70˚C for 10 h. Figure 6 is presented as a line graph, with the horizontal axis representing the nitrocellulose radius (in micrometers) and the vertical axis representing the Butyl-Nena concentration in moles per cubic meter (mol/m^3). In Fig. 6, the concentration profile at 10% (point a) is shown, and a gentle increase in concentration is observed for small to medium radii.

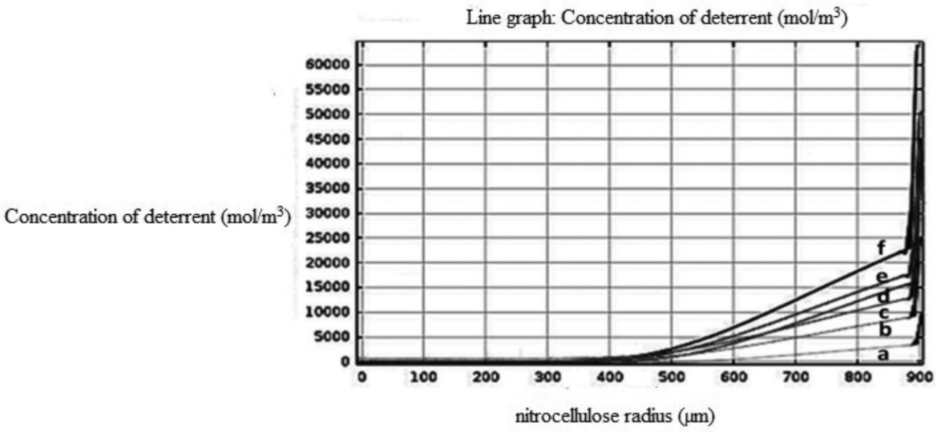

Fig. 5 Concentration profiles of 2–12% polymeric deterrent in terms of nitrocellulose radius at 70˚C for 4 h. (a) 2% polymeric deterrent, (b) 4% polymeric deterrent, (c) 6% polymeric deterrent, (d) 8% polymeric deterrent, (e) 10% polymeric deterrent, (f) 12% polymeric deterrent

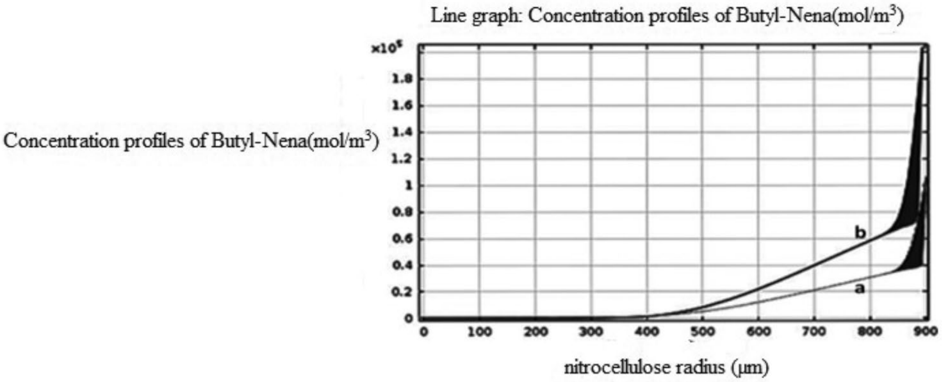

Fig. 6 Concentration profiles of (a) 10 and (b) 20% Butyl-Nena in terms of radius of propellant at 70˚C for 10 h

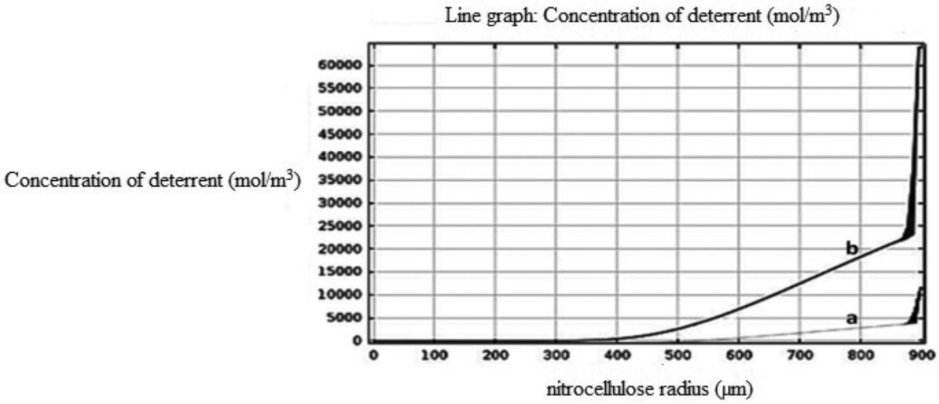

Fig. 7 Concentration profiles of (a) 2 and (b) 12% polymeric deterrent in terms of radius of propellant at 70˚C for 10 h

While the 20% profile (point b) shows a faster and more significant increase in concentration, reaching high values at larger radii. These results indicate a significant effect of Butyl-Nena concentration on its concentration distribution pattern with increasing radius. Figure 6 concentration 10% (point a) A slight increase in Butyl-Nena concentration is observed with increasing nitrocellulose radius. This increase continues up to intermediate radii and then approaches a constant value. Concentration 20% (point b) A more rapid and significant increase in Butyl-Nena concentration is observed with increasing nitrocellulose radius. This increase quickly reaches a maximum value.

Figure 7 shows the concentration profiles of deterrent polymers at two concentrations of 2% and 12%, measured at 70˚C for 10 h. The graph is plotted as a line graph, with the horizontal axis representing the nitrocellulose radius (in micrometers) and the vertical axis representing the deterrent concentration in moles per cubic meter (mol/m^3). In Fig. 7, the deterrent concentration at 2% (point a) gradually increases and reaches significant values, while at 12% (point b), the concentration rapidly approaches a maximum value. These results indicate a significant effect of deterrent concentration on the concentration profiles with increasing radius.

Validation of the simulation

The ageing of coated single base propellants very rarely results in problems: The rates of chemical ageing (regarding stabiliser depletion and nitrocellulose degradation) are very low. Furthermore, the deterrents commonly used for surface coating diffuse very slowly into the single base propellant grains. As a consequence, only minor changes in interior ballistic behaviour occur even under extreme ageing conditions, and both excellent functional life and service life values can be predicted (Fig. 8). On the other hand, it was found that most deterrents diffuse quickly into double base propellants. In one particular case (which is known for its reduced functional life), the deterrent diffusion is so fast that it can be monitored not only at elevated temperatures but even at room temperature (Fig. 9). Furthermore, also the rate of chemical ageing is inherently increased in double base propellants (due to the lower stability of nitroglycerine compared to nitrocellulose). As a consequence, it is very difficult to obtain sufficient functional life and service life values with coated double base propellants for small and medium calibre applications. Figures 8–10 are the results of an experimental work which was doneon a spherical propellant by Vogelsanger et al. [24]. The diffusion process of the experimental work is corresponded with the simulation, but since experimental works carried out in this subject are limited and no experimental work with Butyl-Nena and Polyethylene-Glycol-Dimethacrylatewas found, the study of Vogelsanger et al. [24]was used for validation, but considering that all parameters such as nitrocellulose spherical geometry, radius, the deterrent types used for coating and as a result, the diffusion coefficient differed with the present workparameters, we could not have a point to point comparison betweenthe experimental work and simulation, so, a simulation based on the spherical geometry and the related parameters with Ossola's work was done. As a result, it can be concluded that as the simulation with spherical geometry was so close to the experimental results, the simulation results with cylindrical geometry and considered parameters were reasonable and valid. Figure 11 examines the deterrent concentration profiles in a spherical nitrocellulose and shows two different states of deterrent release"A" diffusion into the spherical propellant. (a) polymeric deterrent "A" diffusion for t0 (un-aged propellant), (b) Polymeric deterrent "A" diffusion at 71˚C for 28 days." As the penetration depth increases, the deterrent concentration "A" decreases significantly and approaches a constant value. In the fresh state (t0), the deterrent is evenly distributed on the surface of the nitrocellulose and the initial concentration is high. This curve shows a uniform distribution of deterrent "A" in fresh nitrocellulose. The deterrent concentration decreases regularly with

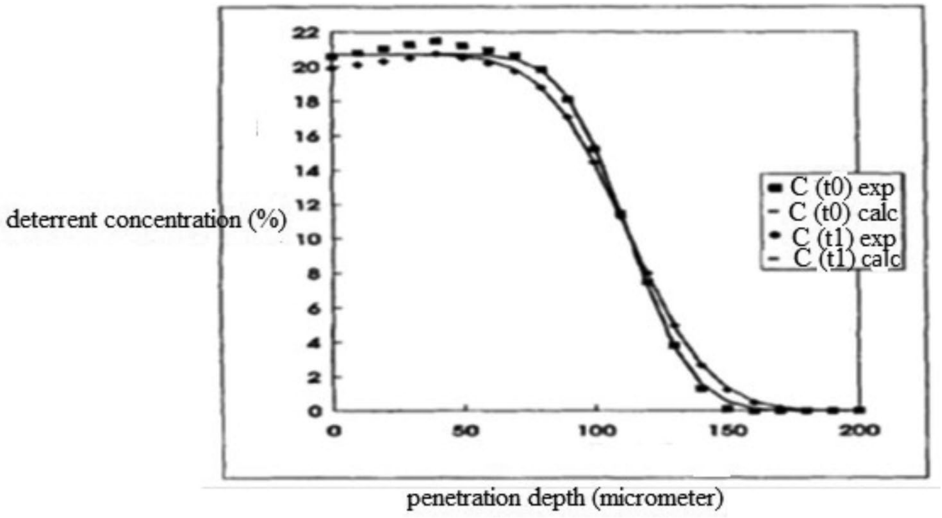

Fig. 8 Concentration profiles of deterrent DBP in a single phase propellant. Measured concentration values (dots) and recalculated concentration profile (lines: obtained by fitting the measured values to the model) for t0 (un-aged propellant) and t1 (propellant stored at 71˚C for 28 days). Fitted D value: 0.05.10–15 m2/s [14]

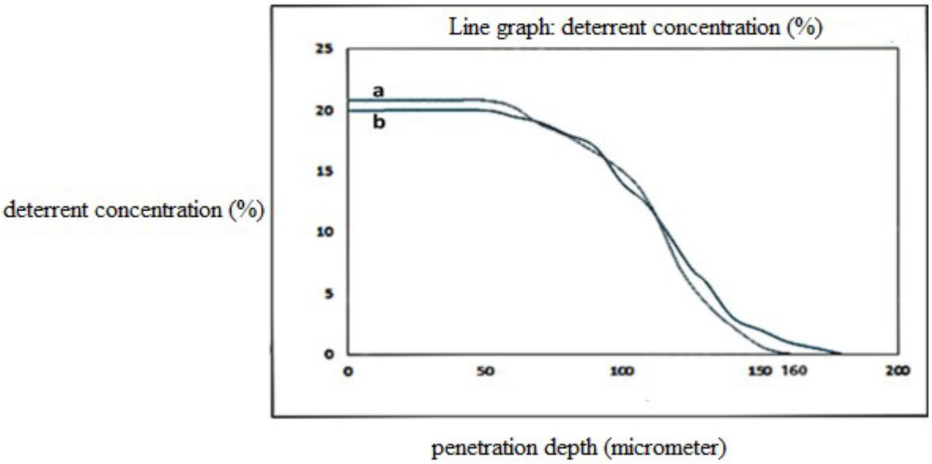

Fig. 9 Resulted diagrams obtained from simulation of DBP deterrent diffusion into the spherical propellant. (a) DBP deterrent diffusion at 70˚C for t0 (un-aged propellant), (b) DBP deterrent diffusion at 71˚C for 28 days

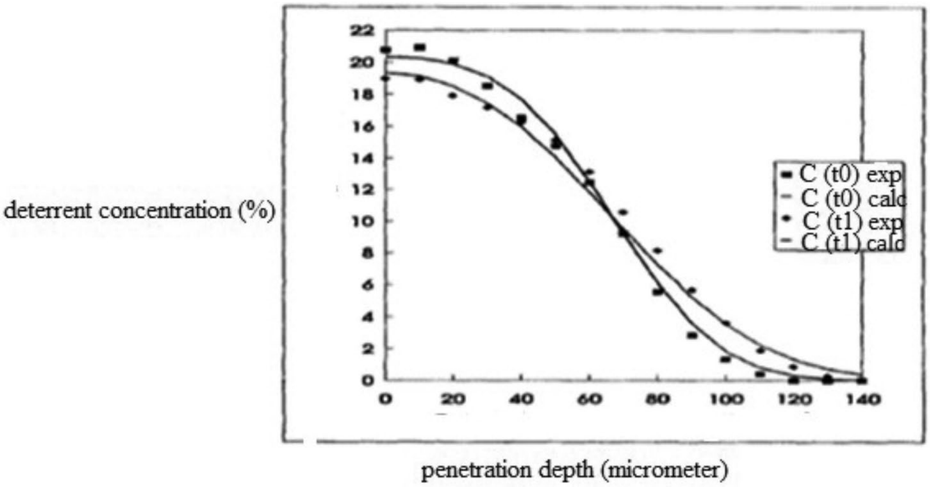

Fig. 10 Concentration profiles of polymeric deterrent "A" in a double based propellant. Measured concentration values (dots) and recalculated concentration profile (lines: obtained by fitting the measured values to the model) for t_0(un-aged propellant) and t_1 (propellant stored at 71˚*C* for 28 days). Fitted D value: $0.13.10^{-15}$ m^2/s [24]

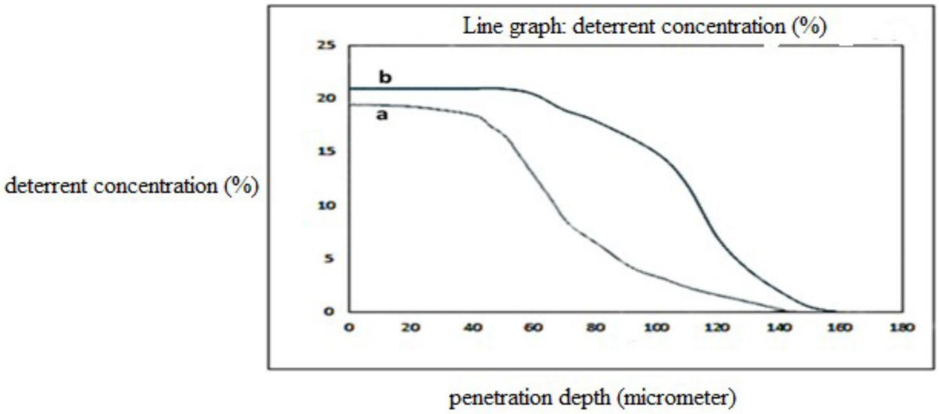

Fig. 11 Resulted diagrams obtained from simulation of DBP deterrent diffusion and the polymeric deterrent "A" diffusion into the spherical propellant. (a) polymeric deterrent "A" diffusion for t_0 (un-aged propellant), (b) Polymeric deterrent "A" diffusion at 71˚C for 28 days

increasing depth, indicating the potential for the impregnants to penetrate the nitrocellulose structure. Increasing temperature and time improves the penetration of deterrent “A” into nitrocellulose. These results can help to better understand the behavior of deterrents under different environmental conditions, which is important for optimizing the development processes and use of polymeric materials. Figure 11 shows the effect of time and temperature on the distribution of deterrents in the nitrocellulose structure, allowing designers and researchers to develop more effective methods for the systematic and optimal use of deterrents in polymer compositions. In the hotter condition, deterrent “A” may penetrate the nitrocellulose more easily and quickly, which is why deterrent concentration is reduced at greater depths, especially compared to the unaged condition.

Conclusion

- In this study, the simulation of deterrent diffusion (Butyl-Nena and Polyethylene-Glycol-Dimethacrylate)in nitrocellulose propellant was performed. Results showed that temperature had greater impact on diffusion depth of both substances rather than concentration and time. As diffusion coefficient of both deterrents is very small, therefore the ultimate diffusion depth differs very low, and this means the excellent diffusion stability of them. These substances remain stable in nitrocellulose, meaning that the propellant efficiency does not decrease during shelf life and aging. So that to achieve the excellent diffusion stability and the best chemical and mechanical properties, these deterrents that used in coating, showed excellent stability in the simulation that is in agree with the experimental goal, keep the propellant launching performance constant and increase in concentration and temperature, does not reduce the efficient life of it over time. Since the particles diffusion process was identical due to validation test, our simulation results will be close to which will be carried out in future.
- Ageing of propellants, in particular the diffusion of surface coatings, has been demonstrated to strikingly influence the functional life of ammunition.
- Knowledge of these processes is therefore essential in order to optimally design the next generation of highest performance propellants for small and medium calibre ammunition.
- It has been proven that, if this knowledge is applied, coated “semi double base” propellants with excellent ballistic performance, combined with sufficient functional life and service life, can be successfully developed and produced.
- Research is under way in order to further improve performance and resistance towards ageing of such propellants. These activities include the substitution of Nitrocellulose by less sensitive energetic plasticizers as well as the search for polymeric deterrents with even lower diffusion potential, including cross-linked polymers.
- Increasing the concentration of Butyl-Nena causes the concentration distribution to increase significantly at larger radii. This indicates the influence of Butyl-Nena concentration on the concentration profile.
- At higher concentrations, Butyl-Nena rapidly penetrates nitrocellulose and reaches higher concentrations penetration depth is higher in aged propellant. This could be due to changes in the polymer structure of the propellant during aging, which increases permeability.
- Restraints are used to control the combustion rate of propellants. By creating a layer with a high concentration of depth on the surface, the burn rate is reduced.
- Heating nitrocellulose to 71 °C and prolonged penetration time affected the deterrent behavior. This indicates an increase in thermal activity and facilitation of the deterrent penetration process.
- As the penetration depth increases, the concentration of deterrent “A” decreases again, but this time with a lower slope and to values lower than the fresh state.
- Increasing the concentration of Butyl-Nena causes a faster and more significant increase in concentration at larger radii.

Author contributions
Hussein Riyadh Abdul Kareem Al-Hetty, Abdulla A. Al-dulaimi, Hiba Muwafaq Saleem: writing—original draft, formal analysis, visualization, methodology, conceptualization, Ehsan Kianfar.: writing—original draft, formal analysis, visualization, methodology, conceptualization, supervision. prepared figures 1-11. All authors reviewed the manuscript.

Funding
This research received no external funding.

Data availability
The datasets used and/or analysed during the current study are available from the corresponding author on reasonable request.

Declarations

Ethics approval and consent to participate
Not applicable.

Consent for publication
Not applicable.

Competing interests
The authors declare no competing interests.

Received: 8 March 2024 / Accepted: 30 April 2025

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