

## CHEMICAL-MATERIAL COMPATIBILITY STUDY WITH INITIAL DECON GREEN FORMULATION

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### ABSTRACT

The army is currently developing Decon Green, a thorough decontaminant intended to be more effective, environmentally friendly, applicable to an extreme temperature range, and more material-compatible than the standard decontaminant DS2. The objective of this study was to compare the effects of Decon Green on thermoplastics and rubbers of military interest with the effects caused by DS2. These effects were observed by comparing physical properties of test specimens before and after exposure to both decontaminants. Percent weight gain, percent extraction, solubility corrected for extraction, rate of decontaminant sorption, and changes in hardness, appearance and volume were noted. It was found that DS2 affected materials to a greater degree than Decon Green.

### INTRODUCTION

The Applied Chemistry Team and the Advanced Chemistry Team, Edgewood Chemical-Biological Center (ECBC), are developing a decontaminant based on peroxydicarbonate and propylene carbonate. The decontaminant Decon Green will be used as a thorough decontaminant and will replace the U.S. Army's standard chemical agent decontaminant DS-2. The objective of the program is to develop a decontaminant that is as effective against chemical and biological agents, applicable to an extreme temperature range, material compatible, and more environmentally acceptable than DS-2. The current formulation consists of propylene carbonate ( $\approx 72.28$  wt %), 50% hydrogen peroxide ( $\approx 24.42$  wt %), Triton X-100 (0.974 wt %), potassium hydrogen carbonate (0.976 wt %), and potassium carbonate (1.35 wt %). This report documents the initial chemical-material compatibility test with Decon Green.

### EXPERIMENTAL METHODS

#### MATERIALS AND CHEMICALS

Propylene carbonate, 50% hydrogen peroxide, Triton X-100, potassium hydrogen carbonate, and potassium carbonate were obtained from Aldrich Chemical Company. DS2, 70% diethylenetriamine, 28% methoxyethanol, and 2% sodium hydroxide, was a laboratory sample. The CB Reference Materials are listed in Table 1.<sup>4, 5, 6</sup>

# Report Documentation Page

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Table 1. Materials Exposed to Decon Green and DS2

SAMPLE	MATERIAL	CODE	SOURCE	USE
1	Polyethylene methylacrylate acrylic acid	PETA	Smithers Scientific	
2	Polyethylene propylene	PEP	Smithers Scientific	M40/M42 mask drink tube
3	Polycarbonate (thermoplastic)	PC	Harbor City Plastics	mask lens
4	Polybromobutyl isoprene	PBB	Smithers Scientific	M43A1 mask faceblank
5	Polyurethane	PU	I. B. Moore	
6	Polyepichlorohydrin	PEH	Smithers Scientific	
7	Polyvinylchloride (thermoplastic)	PVC	Harbor City Plastics	M24/M25A1 mask
8	Polyisoprene	PIP	Smithers Scientific	M17A2 /24 /25A1 mask faceblank
9	Polyphenylene oxide (thermoplastic)	PPO	Harbor City Plastics	M40/42 mask canister component
10	Polydimethylsiloxane	PDMS	Smithers Scientific	M40/42 mask faceblank

## PROCEDURE

Three groups consisting of one replicate of each of the above materials were tested. Samples in groups 1 and 2 were immersed in Decon Green at 49°C, while Group 3 samples were immersed in DS 2. Samples were removed, blotted and weighed at 15 min and 3 h time intervals. Afterwards, samples were allowed to desorb until their masses stabilized. Measurements (mass, length, width, thickness, hardness) were taken before immersion, at the designated intervals, and after desorption. Changes in appearance were noted throughout.

## CALCULATIONS

Equation 1: *Weight gain (WtGn)* = [(wt of specimen + sorbed liquid) - wt of specimen]

Equation 2: *Percent weight-gain (%WtGn)* = Wt gain (100) / Wt of dry specimen

Equation 3: *Extraction (Ext)* = Wt of specimen - wt of desorbed specimen

Equation 4: *Percent extraction (%Ext)* = Extraction (100) / Initial Wt of specimen

Equation 5: *Sorption corrected for Extraction (Scorr%)* = % wt gain + % extraction

## RESULTS AND DISCUSSION

### OBSERVATIONS

Observations on the post-exposure samples are provided in Table 2. When PIP and PBB were immersed in Decon Green, the solution became yellow indicating either a possible chemical reaction or that a component had been extracted from the material; a white residue appeared on the surface of PBB. DS2 and Decon Green either dissolved or degraded polyurethane (PU) within 15 minutes. PPO became tacky after exposure to both Decon Green and DS2. PVC exposed to DS2 changed from creamy white to black. DS2 partially degraded or extracted components from the PDMS sample; however, no degradation or extraction was apparent at the 15-minute weighing. The remaining piece of PDMS was slightly distorted, but pliable.

Table 2. Observations of Chemical-Material Compatibility on Post-Exposure Samples

SAMPLE	GROUP		
	GROUP 1 (Decon Green Exposure)	GROUP 2 (Decon Green Exposure)	GROUP 3 (DS2 Exposure)
PETA	NA	Semi-glossy and tacky	No apparent change
PEP	Glossy, smooth and pliable	Glossy and smooth	No apparent Change
PC	NA	Dull, cloudy, tacky	Dull, cloudy, tacky. Blue hue changed to violet
PBB	Dull, pliable, white residue	White residue, but no residue	No apparent change
PU	NA	Dissolved in 15 min	Dissolved in 15 min
PEH	Tacky with swelling	Tacky with swelling	Brittle, less pliable.
PVC	No apparent change	No apparent change	Color change from white to black
PIP	Dull, but no other noticeable changes	Dull, but no other noticeable changes	No apparent change
PPO	Tacky	Tacky	Tacky
PDMS	No apparent change	No apparent change	Some of material dissolved

Notes:

NA = not available

49 degrees Celsius for 3 hours and 15 minutes

#### PERCENT WEIGHT-GAIN

The percent weight-gain for each material in each group and the average for Decon Green replicates at 3 h are provided in Table 3. Decon Green and DS2 either dissolved or degraded PU, and DS2 dissolved PC during the sorption tests. All of the other samples experienced weight gain during the sorption process, except for the PDMS sample exposed to DS2. In most cases, samples exposed to DS2 had a greater percent weight-gain than samples exposed to Decon Green. PEH samples experienced the highest percentage of weight gain among samples in both the DS2 group and the Decon Green group.

Table 3. Percent Weight-Gain for Materials Exposed to Decon Green and DS2

Material	GROUP			
	1 (Decon Green Exposure)	2 (Decon Green Exposure)	Ave 1 & 2	3 (DS2 Exposure)
PETA	NT	27.77	27.77	18.15
PEP	0.41	0.79	0.60	1.83
PC	NT	0.32	0.32	dissolved
PBB	0.70	0.88	0.79	1.84
PU	Dissolved or degraded	Dissolved or degraded	NA	Dissolved or degraded
PEH	49.33	51.25	50.29	91.31
PVC	0.49	0.64	0.57	4.67
PIP	0.87	1.12	1.00	5.88
PPO	0.39	0.48	0.44	0.50
PDMS	0.55	0.29	0.42	-30.72

Notes:

NT=not tested

NA= not available

Ave=average

49 degrees Celsius for 3 hours

PERCENT EXTRACTION

The percent extraction values for the materials within each group are provided in Table 4. The average of Group 1 and Group 2 is also provided in Table 4. Most materials exposed to DS2 and Decon Green did not have percent extraction values of more than 2%. The percent extraction values for DS2 samples tended to be negative, indicating that the samples were not fully desorbed, although their masses had stabilized. The samples exposed to Decon Green tended to have positive percent extraction values; indicating that the specimens had either been degraded or components were extracted during the sorption process.

Table 4. Percent Extraction for Materials Exposed to Decon Green and DS2

Material	GROUP			
	1 (Decon Green Exposure)	2 (Decon Green Exposure)	Ave 1 & 2	3 (DS2 Exposure)
PETA	NT	4.86	4.86	-5.51
PEP	0.18	-0.12	0.03	-1.35
PC	NA	0.76	0.76	NA
PBB	0.40	0.63	0.52	-0.18
PU	NT	NT	NA	NT
PEH	0.79	1.62	1.21	-34.14
PVC	-0.09	-0.21	-0.15	-2.08
PIP	1.18	1.72	1.45	-1.91
PPO	0.02	0.01	0.02	-0.04
PDMS	0.11	0.42	0.27	**32.64

Notes:

NT=not tested

NA=not available

Ave is average

\*\*PDMS was either partially dissolved or degraded by DS2

49 degrees Celsius for 3 hours

SORPTION CORRECTED FOR EXTRACTION

The sorption-corrected percents for the materials within each group are provided in Table 5. Because each material (excluding PDMS, PC, and PU) exposed to DS2 and PEP (Group 2) and PVC (Groups 1 and 2) had a negative percent extraction, the sorption-corrected percent for those materials is just the percent weight-gain. Typically, sorption-corrected percents were larger for DS2-exposed samples than for Decon Green-exposed samples. The highest sorption-corrected percentages were observed for the PEH samples exposed to either decontaminant.

Table 5. Sorption-Corrected Percent for Materials Exposed to Decon Green and DS2

Material	GROUP			
	1 (Decon Green Exposure)	2 (Decon Green Exposure)	Ave 1 & 2	3 (DS2 Exposure)
PETA	NT	32.63	32.63	18.15
PEP	0.60	0.79	0.70	1.83
PC	NT	1.08	1.08	NT
PBB	1.11	1.51	1.31	1.84
PU	NT	NT	NA	NT
PEH	50.12	52.87	51.50	91.31
PVC	0.49	0.64	0.57	4.67
PIP	2.05	2.84	2.45	5.88
PPO	0.41	0.49	0.45	0.47
PDMS	0.66	0.71	0.69	1.92

Notes:

NT=not tested

NA=not available

Ave =average

49 degrees Celsius for 3 hours

#### PERCENT CHANGE IN INDENTATION HARDNESS

The percent change in hardness for each material is provided in Table 6. Percent change in hardness values were varied between the two groups of samples exposed to Decon Green; the reason is unknown. The majority of samples from Group 1 experienced negative changes in hardness, indicating that the post-exposure hardness values were less than the pre-exposure hardness values. In contrast, the samples from Group 2 had positive changes in hardness after being exposed to Decon Green indicating that the post-exposure hardness values were greater than pre-exposure hardness values. PDMS from Group 2 had the greatest change, but the initial hardness value of this particular PDMS sample was nearly half the initial hardness value of other PDMS samples. Increases in hardness were observed for PETA, PVC, PIP, PPO and PDMS exposed to DS2. The other Group 3 samples experienced decreases.

Table 6. Percent Change in Hardness for Materials Exposed to Decon Green and DS2

Material	GROUP			
	1 (Decon Green Exposure)	2 (Decon Green Exposure)	Ave 1 & 2	3 (DS2 Exposure)
PETA	NT	15.17	15.17	14.01
PEP	-0.74	20.43	9.85	-0.67
PC	NA	10.21	10.21	NA
PBB	-0.45	7.37	3.46	-0.28
PU	NT	NT	NA	NT
PEH	-2.06	12.55	5.25	-53.02
PVC	-0.96	7.49	3.27	7.50
PIP	-0.69	26.49	12.9	27.78
PPO	-1.79	5.99	2.10	6.39
PDMS	-0.56	70.24	34.84	7.29

Notes:

NT=not tested

NA=not available

Ave=average

49 degrees Celsius for 3 hours

#### PERCENT CHANGE IN VOLUME

Both Decon Green and DS2 caused changes in the dimensions of the samples tested. The majority of samples tested with these decontaminants experienced a decrease in overall volume after exposure. The change in volume percentage for each material is provided in Table 7. Every sample tested in Group 1 experienced a decrease in volume except PEP, which had an increase. The greatest decrease in volume of Group 1 samples was observed for PBB. PEP and PVC were the only Group 2 samples that had an increase in volume after exposure to Decon Green. The greatest decrease among Group 2 samples was observed for PDMS, which had a volume decrease of  $\approx 30\%$ . In Group 3, only PEH and PVC had positive changes in volume. PEH experienced the greatest increase. PDMS had the largest decrease in volume among samples exposed to DS2.

Table 7. Percent Change in Volume for Materials Exposed to Decon Green and DS2

Material	GROUP			
	1 (Decon Green Exposure)	2 (Decon Green Exposure)	Ave 1 & 2	3 (DS2 Exposure)
PETA	NT	-19.90	-19.90	-4.08
PEP	0.59	4.90	2.75	-1.50
PC	NA	-1.29	-1.29	NA
PBB	-22.35	-23.66	-23.00	-21.18
PU	NT	NT	NA	NT
PEH	-16.09	-22.14	-19.12	56.57
PVC	-1.34	0.03	-0.66	7.78
PIP	-13.05	-20.29	-16.67	-22.62
PPO	-0.99	-1.82	-1.41	-1.70
PDMS	-22.25	-29.61	-25.93	-41.91

Notes:

NT=not tested

NA=not available

Ave=average

49 degrees Celsius for 3 hours

#### SORPTION AS A FUNCTION OF SURFACE AREA AND TIME

The amount of DS2 and Decon Green sorbed by each material was calculated as a function of surface area per time. The calculations were made for two time intervals, 15 and 180 minutes. The two Decon Green trials (Groups 1 and 2) were averaged together for these calculations. The results are provided in Table 8. The amount of Decon Green and DS2 absorbed by PPO at 15 and 180 minutes, respectively, were similar. The masses of DS2 absorbed by PBB and PEH were approximately twice the amount of Decon Green absorbed by the materials at each time interval. The amount of DS2 absorbed by PEP after 3 h was about 2.5 times the mass of Decon Green sorbed. At 180 minutes, the mass of DS2 absorbed by PVC was a factor of eight greater than the amount of Decon Green absorbed. PIP absorbed more DS2 than Decon Green by a factor of six (t = 180 min).

Table 8. Mass of Decontaminant Absorbed Per Surface Area and Time

MATERIAL	DECONTAMINANT			
	<sup>a</sup> Decon Green		DS2	
	$\mu\text{g}/\text{cm}^2$ at 15 min	$\mu\text{g}/\text{cm}^2$ at 180 min	$\mu\text{g}/\text{cm}^2$ at 15 min	$\mu\text{g}/\text{cm}^2$ at 180 min
PETA	2919.5	14963.2	2276.5	9869.7
PEP	98.7	322.7	265.6	789.5
PC	281.6	340.5	NA	NA
PBB	146.7	425.8	266.3	945.5
PU	NA	NA	NA	NA
PEH	4338.7	32930.4	8282.0	60612.3
PVC	302.1	683.6	913.9	5700.5
PIP	245.3	492.7	578.4	2942.7
PPO	363.7	422.1	320.3	447.1
PDMS	103.6	144.3	NA	NA

Notes:

<sup>a</sup>The Decon Green value is the average of Group 1 and Group 2.

NA=not available

## CONCLUSIONS

Most materials were affected to a greater degree by exposure to DS2 than to Decon Green. DS2 dissolved PC and PU, and partially degraded or extracted PDMS. Decon Green dissolved only PU. Materials exposed to DS2, which were not dissolved or degraded, did not completely desorb even at 70 °C. The only material that did not completely desorb when exposed to Decon Green was PVC. Other materials (PEP, PEH, PVC, PIP) absorbed greater amounts of DS2 than Decon Green. Only PETA absorbed more Decon Green than DS2.

The difference in hardness of the materials after exposure to the two decontaminants is more difficult to evaluate because of inconsistency between Group 1 and Group 2. Typically, the change in hardness was positive for Group 3 (except PEP, PBB, and PEH), Group 2, and the average of Groups 1 and 2.

Typically, materials exposed to DS2 and Decon Green had a negative change in volume. Only PEP (Groups 1 and 2), PEH and PVC (Group 3) had an increase in volume. PEH, PVC, and PDMS when exposed to DS2 had a much larger increase in volume than the samples exposed to Decon Green. Only PETA (Group 2) had a much larger change in volume than PETA exposed to DS2.

Based on the positive trend in the sorption values (Table 8), all materials had not reached equilibrium after 3 h. Therefore, larger exposure times to the decontaminants would cause more severe effects in the materials.

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