Permeation of a malathion formulation through butyl gloves

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Abstract

The factors that determined the permeation kinetics of a commercial malathion formulation (Prent) and its reconstituted cocktail of malathion and its xylene-range fraction inert ingredients at Prent concentrations (Recon) were investigated for an unlined unsupported butyl industrial type glove in an ASTM-type permeation cell with liquid 2-propanol collection and subsequent analysis by gas chromatography/mass spectrometry. For both Prent and Recon, the steady-state permeation rate P_s correlated inversely with the logarithm of the breakthrough time t_b, as did $\log P_s$ with $\log t_b$. P_s, $\log P_s$, P_s/t_1 and $\log P_s/t_1$ (where t_1 is the lag time) versus the logarithm of the weight percentage of component divided by the total weight were linear too. After accounting for mixture composition, the second strongest linear regression term was liquid molar volume, and the strongest third term was octanol–water partition coefficient ($\log K_{ow}$). Retention volumes, $V_R(t_1)$ at t_1 and $V_R(t_{s1})$ at the first observed time in the steady-state t_{s1} of each chemical in Prent and Recon, were also similarly correlated to the weight percentage and $\log K_{ow}$ or Snyder elution strength (E^o). At least three independent variables are necessary to account for the permeation of this complex mixture. One factor accounts for composition, another for molecular size, and the third for partitioning behavior. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

The major route of human exposure to nonvolatile pesticides is through the skin [1]. Workers must wear the correct glove for adequate protection against not only the

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pesticide but also the liquid components of pesticide formulations since the latter may control pesticide permeation [2]. The most used industrial glove is nitrile followed by butyl [1].

Butyl rubber is a copolymer of isobutylene and isoprene [1]. The isoprene is linked predominantly by 1,4-addition at a level from 0.5 to 2.5 mol per 100 mol of monomers; the residual olefin is about 1:1 *cis* to *trans* ratio [3]. Butyl rubber is made by precipitation polymerization in which a feed stock of isobutylene and isoprene in an inert diluent like methyl chloride at about -100 to $-90°C$ is fed into a large well-agitated reactor; chilled aluminum chloride and a trace of water at about $-95°C$ are added as catalysts [3,4]. Upon contact of feed and catalyst, the polymer is formed by a highly exothermic reaction [4]. The heat of reaction is about 10 kcal/mol [4]. The rubber has good resistance to light and ozone, excellent flexing properties, excellent heat resistance, and good tensile and tear resistances [1]. It exhibits excellent resistance to corrosive chemicals, vegetable oils, phosphate ester oils, and some ketones [1,5]. Butyl gloves also exhibit permeation resistance to water vapor [5]; water is the most common carrier used to dilute pesticide emulsion concentrates for field spraying. The butyl gloves of different manufacturers differ in their barrier properties.

Swedish butyl gloves were degraded by cumene (CAS Number: 98-82-8) and diethylbenzene (CAS Number: 25304-17-4) [6]. Degradation was also observed when technical xylene (CAS Number: 1330-20-7) challenged butyl gloves (North, B-161, 0.65 mm) [6]. The breakthrough times (t_b)- steady-state permeation rates (P_s) for *m*-xylene (CAS Number: 108-38-3) and *o*-xylene (CAS Number: 95-47-6) for butyl gloves (North, B-174, 0.67 mm and 0.63 mm) were 39 min-876 mg/m²-min, and 52 min-1164 mg/m²-min, respectively [6]. A study of 76% ethyl parathion formulated in 10% total xylenes for butyl gloves (thickness = 0.48 mm) reported that *m*-xylene did not break through before 480 min [7]. When the same butyl gloves were challenged with 43% methyl parathion formulated in 48% xylenes, the t_b range of *m*-xylene was 120–180 min [7]. The t_b range of *m*-xylene through the same butyl gloves was 30–120 min if the challenge solution was endosulfan formulation (nominal contents: 34% endosulfan and 57% xylenes) [7]. Xylene range chemicals are inert components in many malathion emulsion concentrate pesticide formulations [8].

The chromatographic model of permeation predicts that $\log t_i$ (t_i is the lag time t_1, where the extrapolated steady state section corresponds to a permeated concentration of zero, or $\log t_b$) are linearly related to the Snyder elution strength $E°$, the latter being correlated to the logarithm of the octanol/water coefficient, $\log K_{ow}$ [9]. The dependence of permeation characteristics on retention volume V_R using chromatographic theory is [8,9]:

$$V_R = P_s A t_R / d \tag{1}$$

where: V_R: the retention volume of the analyte; t_R: the lag time (t_1) or the first time point of the steady-state period (t_{s1}); P_s: the steady-state permeation rate for the analyte (mass/area–time); A: cross-sectional area of the exposed gloves; d: the density of the analyte (mass/volume).

A related model, the liquid–liquid partition model, has also been proposed [9]. To permeate, a solute must successfully pass through hydrophobic and hydrophilic obsta-

cles. Many gloves consist of an elastomer coated by films of different polarities to protect against both aqueous solutions and hydrophobic compounds [1]. The situation can be described by the partition coefficients, K_{sw} of a solute between an organic solvent and water in terms of the equilibrium concentration of analyte in a reference organic solvent (C_s) and the equilibrium concentration of analyte in water of the same volume as the organic solvent (C_w) in Eq. (2):

$$K_{sw} = C_s / C_w \tag{2}$$

The major K_{sw} are for 1-octanol/water (K_{ow}), diethyl ether/water (K_{dw}), *n*-butyl acetate/water (K_{bw}), chloroform/water (K_{cw}), *n*-heptane/water (K_{hw}) [10]. The most values are available for $\log K_{ow}$; $\log K_{hw}$ has a better correlation with E^o than $\log K_{ow}$ [9].

We have reported the permeation kinetics of a malathion formulation through nitrile gloves [8]. The chromatographic model and liquid–liquid partition model were both applicable after accounting for formulation composition and individual molar volumes. The present study investigated whether the permeation kinetics of the same malathion formulation through butyl gloves could be characterized similarly.

2. Experimental

2.1. Gloves and chemicals

The gloves were unlined unsupported butyl from North Hand Protection (Charleston, SC, catalog No. B131, light weight, 0.36–0.38 mm thickness and 28 cm in length). Prentox Malathion 50% Emulsifiable Insecticide™ or 'Prent' (Prentiss Drug and Chemical, Sanderville, GA) contained 50% (w/w) malathion and 50% xylene range aromatic solvents as inert components. The reconstituted solution containing malathion and the xylene-range inert components at the same concentrations as in Prent is hereafter termed 'Recon'. 2-Propanol (Optima) from Fisher Scientific (Fair Lawn, NJ) was the collection medium. Sodium dichromate (Fisher Scientific) was used to generate a known relative humidity atmosphere for glove conditioning. Malathion of 95% nominal purity (Pfaltz and Bauer, Waterbury, CT), *m*-xylene (Kodak, Rochester, NY) and *o*-xylene (Fisher Scientific) were used. The following alkylbenzene molecular weight 120 isomers with indicated nominal purity were from Aldrich Chemical (Milwaukee, WI): *iso*-propylbenzene 99%, *n*-propylbenzene 98%, 3-ethyltoluene 99%, 4-ethyltoluene 99%, and 1,2,3-trimethylbenzene 99%; 1,2,4-trimethylbenzene 99% was from Sigma (St. Louis, MO); 1,3,5-trimethylbenzene 99% was from Eastman Kodak; and *m*-diethylbenzene 98% was from Chemical Service (Westchester, PA). The internal standard, *o*-diethylbenzene (95%) was from Fluka Chemical (Ronkonkoma, NY). All standards were tested for purity by gas chromatography/mass spectrometry (GC/MS).

2.2. Apparatus

ASTM-type I-PTC-600 permeation cells were from Pesce Lab Sales (Kennett Square, PA). The moving tray shaker water bath used for immersion of three permeation cells

simultaneously was a Fisher Scientific model 125 No. 429. Three copper metal tubes (23 cm × 15 mm o.d. × 13.3 mm i.d.) were mounted on the two rails of the shaker after hacksawing the 1 mm wide grooves in the bars and using emery paper to smoothe the jagged edges. Three-prong clamps allowed suspension of three permeation cells above and into the bath water as desired. A micrometer screw gauge (L.S. Starrett, Athol, MA) was used to measure glove thickness before and after experiments. Vernier calipers (Mitutoyo, Japan) allowed measurement of the glove diameters cut for permeation studies. A torque wrench (Mechanics Products, Kent, WA) ensured equal tightness of permeation cell nuts.

The analysis utilized a Hewlett-Packard 5890A gas chromatograph (GC) interfaced with a Hewlett-Packard 5988A quadrupole mass spectrometer (MS). The fused silica capillary column was a J&W Scientific/Alltech (Deerfield, IL), 30 m long × 0.32 mm i.d. DB-1701 with 1.0 μm chemically bonded 14% cyanopropylphenyl film. The MS was operated in the 70 eV positive ion electron impact mode. The helium carrier gas of 99.9999% purity was from Alphagaz (Walnut Creek, CA).

2.3. Methods

The identification and quantification of the inert components and malathion contained in Prent are given elsewhere [8] as are the permeation experimental procedures [2,8] and those for GC/MS analyses [8]. Aliquots of 100-μl were sampled every 20–40 min over 8-h from the collection side of the permeation cell and stored at $-20°$C. A 2-μl aliquot of thawed sample collected was injected into the GC/MS by the sandwich technique. For each single permeation test, 16 samples were taken. The total samples collected were 96 for Prent and Recon in triplicate and 12 compounds were analyzed for each single sample. Thus there were 1152 data points. Backpermeation of 2-propanol into the challenge side liquid and headspace was ascertained at a solvent delay time of zero.

Internal standard calibration curves of each component were performed for each analysis day. The GC/MS linear ranges for the inert components were from 0.5 ng to 18 ng injected mass, while the range for malathion was 4.6 ng to 230 ng. The total permeated mass of each component in the collection medium was calculated from the mass in the 2-μl injection using the internal standard (o-diethylbenzene) method, corrected for fraction injected and for volume sampled previously. Cumulated permeated mass was plotted versus sampling time. The calculations for steady-state permeation rate (P_s), lag time (t_1), and diffusion coefficient (D_p) are given elsewhere [2,11]. The thickness of each glove was measured five times before and after the permeation test by a micrometer screw gauge.

The kinetic parameters were then intercorrelated and correlated to the known w/w percentages (%) in Table 1 [8] with specific combinations through linear–linear, log–linear, linear–log, and log–log analyses. These results were then compared for Prent and Recon. Corresponding nonsignificantly different data at $p \leq 0.05$ were pooled, the process repeated to produce a single correlation equation obeyed by both Prent and Recon for the dependent and independent variables concerned. The same process was performed on individual run data. The equations were then used for further

Table 1
W/W Percentages and selected physical parameters for the chemicals in Prentox™ malathion formulation

Compounds	%	MW	d	MV	$\log K_{ow}$	S_w	DM	E^o
m-Xylene	1.5	106	0.864	123	3.33	160	1.00	0.251
o-Xylene	0.93	106	0.880	121	3.25	221	2.07	0.255
Cumene	2.1	120	0.862	139	3.89	50	0.40	0.218
n-Propylbenzene	2.6	120	0.862	139	3.71	60	0.35	0.228
3-Ethyltoluene	13	120	0.865	139	3.88	94	0.33	0.218
4-Ethyltoluene	4.3	120	0.861	139	3.90	95	0	0.217
Mesitylene	3.3	120	0.865	139	3.78	48	0.13	0.224
2-Ethyltoluene	3.0	120	0.881	136	3.53	93	0.56	0.239
1,2,4-Trimethylbenzene	13	120	0.876	137	3.82	57	0.30	0.222
1,2,3-Trimethylbenzene	0.64	120	0.894	134	3.70	75	0.56	0.229
m-Diethylbenzene	1.0	134	0.860	156	4.44	1.21	0.36	0.185
Malathion	52	330	1.21	273	2.89	145	2.00	0.277

%: Weight percentage of each component in Prent and Recon from GC/MS analyses; MW: Molecular weight in g/mol; d: Liquid density at 20°C; MV: Molar volume in ml/mol at 20°C, calculated by MW/d; $\log K_{ow}$: The logarithm to base 10 of the octanol/water partition coefficient at 25°C; S_w: Water solubility in mg/l at 25°C. The S_w of mesitylene and m-diethylbenzene were estimated by the authors; DM: Dipole moment of the liquid at 20–30°C in Debye; E^o: Snyder elution strength, calculated from $\log K_{ow} = -17.0E^o + 7.59$.

model building to determine the contributions of the known physical constants, molecular weight (MW), liquid density (d), molar volume (MV), K_{ow} [12,13], water solubility (S_w) [12,13], dipole moment (DM) [14,15], and E^o (Table 1) of the Recon chemicals to the residual intercept. The physical constant of highest power was then selected by p-values. The process was then repeated until addition of more terms caused no further significant improvement in p. This resulted in an averaged multivariate regression equation for both Recon and the data of the formulation that agree with those of Recon.

Regression analyses were performed using Microsoft® Excel version 5.0. Tests of statistical significance were at $p \leq 0.05$, using the F-test. The calculated $F = (SS_R/k)/(SS_E)/(n-k-1)$ (where SS_R is the regression sum of squares and SS_E is the residual sum of squares), to be compared with the Table $F_{[1-p;k,n-k-1]}$, for $p \leq 0.05$, where k is the degrees of freedom due to the regression, $n-k-1$ is the degrees of freedom due to the error and n is the number of observations [16]. The correlation coefficient r and probability p-values will be reported.

3. Results and discussion

3.1. Swelling of glove material and backpermeation

The average initial glove thickness did not significantly differ for the two permeation challenges at $p \leq 0.05$, the initial average glove thickness being 0.38 ± 0.02 mm. No permanent swelling of glove materials occurred. Back permeation of 2-propanol also did not happen.

3.2. Kinetic parameters

Tables 2 and 3 show the individual run data, the arithmetic means and their standard deviations (SD) for t_b, t_1, P_s, and D_p for each component in Prent and Recon. Most of the coefficients of variation (CV) are less than 25%. Exceptions are the P_s of n-propylbenzene (CV = 27%), 4-ethyltoluene (CV = 38%), and malathion (CV = 34%) in Prent; m-xylene (CV = 27%), 2-ethyltoluene (CV = 26%), m-diethylbenzene (CV = 25%) and malathion (CV = 31%) in Recon; and the D_p of m-xylene (CV = 28%) in Prent. Most of the corresponding parameters for Prent and Recon at $p \leq 0.05$ differed significantly except for malathion, the major component. All Recon average t_b for the inert components were the same for Prent, excepting m-xylene, n-propylbenzene, and 4-ethyltoluene, which were significantly longer. Recon t_1 increased relative to Prent t_1 excepting m-xylene which decreased. D_p was inversely related to t_1. Most P_s did not differ except 3-ethyltoluene and m-diethylbenzene decreased, and 4-ethyltoluene and 1,2,4-trimethylbenzene increased.

The t_b (60–100 min) for xylenes and trimethylbenzenes were longer than those of the pure chemicals [6], as occurred when this malathion formulation challenged nitrile gloves [8]. The t_b for all components in each challenge medium were also the same, the average t_b for Prent and Recon being 67 ± 6.7 min (CV = 10%) and 83 ± 5.6 min (CV = 6.7%) respectively, both shorter than for nitrile gloves [8]. Prent and Recon Butyl t_b values differed statistically at $p \leq 0.05$. The average t_1 for Prent and Recon were 80 ± 40 min (CV = 50%) and 110 ± 15 min (CV = 14%) respectively, also shorter than for nitrile [8]. These t_1 did not differ at $p \leq 0.05$. Nitrile gloves offer better protection than butyl gloves for this formulation relative to t_b. The respective average P_s for Prent and Recon were 3.8 ± 3.4 $\mu g/cm^2$-min (CV = 90%) and 3.3 ± 3.7 $\mu g/cm^2$-min (CV = 110%) were lower than for nitrile [8]. Thus relative to P_s, butyl gloves are more protective than nitrile.

3.3. Intercorrelation analyses of kinetic parameters

For Prent, the correlation analyses of the kinetic parameters based on the averaged data of Tables 2 and 3 produced 20 relationships at $p \leq 0.05$, all also seen for Recon. The strongest relationships for the averaged data were:

$$\log(P_s) = -6.2\log(t_b) + 12 \quad r = -0.694(p = 0.012) \tag{3}$$

$$\log(t_b/t_1) = -0.0038t_1 + 0.25 \quad r = -0.981(p = 1.8 \times 10^{-8}) \tag{4}$$

$$\log(t_b/t_1) = 1.0\log(D_p) - 0.60 \quad r = -0.955(p = 1.3 \times 10^{-6}) \tag{5}$$

The strongest correlation between D_p and t_1 was:

$$\log(D_p) = -0.98\log(t_1) + 2.4 \quad r = -0.999(p = 3.7 \times 10^{-16}) \tag{6}$$

Note to Table 2:

t_b: Breakthrough time; P_s: Steady-state permeation rate; t_1: Lag time; D_p: Diffusion coefficient (calculated from $t_1 = l^2/6D_p$); The mean data are expressed in the form of arithmetic mean $\pm$ standard deviation.

Table 2

Individual and averaged data for Prentox™ malathion formulation challenge through unlined unsupported butyl gloves (average initial thickness for three runs = 0.39 ± 0.02 mm)

Compound	t_b (min)	P_s (μg/cm^2-min)	t_l (min)	D_p (mm^2/min $\times 10^{-4}$)
m-Xylene	60	2.47	167	1.65
	60	2.83	217	1.15
	60	2.75	229	0.976
Mean $\pm$ Standard deviation	60 ± 0	2.62 ± 0.14	204 ± 33	1.26 ± 0.35
o-Xylene	80	1.22	77.3	3.56
	60	1.47	72.4	3.45
	60	1.18	60.8	3.68
Mean $\pm$ Standard deviation	67 ± 12	1.29 ± 0.16	70.2 ± 8.5	3.56 ± 0.12
Cumene	80	1.50	80.8	3.41
	60	1.72	70.8	3.53
	80	1.62	66.7	3.36
Mean $\pm$ Standard deviation	73 ± 12	1.61 ± 0.11	72.8 ± 7.2	3.43 ± 0.09
n-Propylbenzene	60	3.79	77.5	3.55
	60	2.49	50.9	4.90
	60	4.33	61.1	3.66
Mean $\pm$ Standard deviation	60 ± 0	3.54 ± 0.95	63.2 ± 13.4	4.04 ± 0.75
3-Ethyltoluene	60	11.8	70.5	3.91
	60	10.1	54.7	4.56
	60	10.6	61.0	3.67
Mean $\pm$ Standard deviation	60 ± 0	10.8 ± 0.90	62.1 ± 8.0	4.05 ± 0.46
4-Ethyltoluene	60	6.55	78.2	3.52
	60	7.06	60.2	4.15
	60	3.14	47.9	4.68
Mean $\pm$ Standard deviation	60 ± 0	5.58 ± 2.13	62.1 ± 15.3	4.14 ± 0.58
Mesitylene	60	3.98	82.1	3.35
	80	3.89	69.6	3.58
	80	3.61	67.5	3.52
Mean $\pm$ Standard deviation	73 ± 12	3.83 ± 0.19	73.1 ± 7.9	3.42 ± 0.14
2-Ethyltoluene	80	2.39	79.3	3.47
	60	2.58	81.2	3.07
	60	1.78	52.1	4.30
Mean $\pm$ Standard deviation	67 ± 12	2.25 ± 0.42	70.9 ± 16.3	3.61 ± 0.62
1,2,4-Trimethylbenzene	60	9.38	70.8	3.89
	60	11.1	58.1	4.29
	60	9.97	56.3	3.89
Mean $\pm$ Standard deviation	60 ± 0	10.1 ± 0.85	61.7 ± 7.9	4.05 ± 0.21
1,2,3-Trimethylbenzene	80	0.465	82.3	3.35
	60	0.479	61.6	4.05
	80	0.466	71.4	3.14
Mean $\pm$ Standard deviation	73 ± 12	0.470 ± 0.008	71.7 ± 10.3	3.51 ± 0.48
m-Diethylbenzene	80	1.70	79.9	3.44
	60	1.76	66.6	3.74
	60	1.60	63.5	3.53
Mean $\pm$ Standard deviation	67 ± 12	1.69 ± 0.08	70.0 ± 8.7	3.57 ± 0.15
Malathion	80	1.04	83.6	3.29
	80	1.83	88.0	2.84
	80	1.07	58.1	3.86
Mean $\pm$ Standard deviation	80 ± 0	1.31 ± 0.45	76.6 ± 16.2	3.33 ± 0.51

Table 3
individual and averaged data for the reconstituted cocktail challenge (malathion plus Prent alkylbenzenes) through unlined unsupported butyl gloves (average initial thickness for three runs = 0.36 ± 0.02 mm).

Compound	t_b (min)	P_s ($\mu g/cm^2 - min$)	t_1 (min)	D_p ($mm^2/min \times 10^{-4}$)
m-Xylene	80	3.29	111	2.27
	80	2.01	99.3	1.94
	80	3.39	117	1.87
Mean ± Standard deviation	80 ± 0	2.90 ± 0.77	109 ± 9	2.03 ± 0.22
o-Xylene	80	1.52	117	2.14
	80	0.982	96.6	1.99
	80	1.48	109	2.00
Mean ± Standard deviation	80 ± 0	1.32 ± 0.29	108 ± 11	2.05 ± 0.08
Cumene	80	2.34	133	1.89
	100	1.48	109	1.77
	80	2.27	123	1.79
Mean ± Standard deviation	87 ± 12	2.03 ± 0.48	122 ± 12	1.81 ± 0.06
n-Propylbenzene	80	2.71	121	2.08
	100	1.90	108	1.78
	80	2.69	111	1.96
Mean ± Standard deviation	87 ± 12	2.43 ± 0.46	113 ± 7	1.94 ± 0.15
3-Ethyltoluene	60	8.61	90.5	2.78
	80	7.64	80.7	2.36
	80	9.55	87.9	2.49
Mean ± Standard deviation	73 ± 12	8.60 ± 0.96	86.4 ± 5.1	2.55 ± 0.21
4-Ethyltoluene	80	3.09	100	2.53
	80	3.08	91.1	2.11
	80	2.99	104	2.11
Mean ± Standard deviation	80 ± 0	3.05 ± 0.06	98.4 ± 6.6	2.25 ± 0.24
Mesitylene	80	1.31	87.8	2.87
	100	1.35	91.4	2.10
	80	1.34	85.4	2.56
Mean ± Standard deviation	87 ± 12	1.33 ± 0.02	88.2 ± 3.0	2.51 ± 0.39
2-Ethyltoluene	80	1.81	119	2.12
	100	1.62	113	1.69
	80	2.60	123	1.78
Mean ± Standard deviation	87 ± 12	2.01 ± 0.52	118 ± 5	1.86 ± 0.22
1,2,4-Trimethylbenzene	80	13.7	101	2.49
	60	11.2	94.3	2.04
	80	14.5	90.2	2.43
Mean ± Standard deviation	73 ± 12	13.1 ± 1.7	95.1 ± 5.5	2.32 ± 0.25
1,2,3-Trimethylbenzene	80	0.425	103	2.45
	100	0.394	108	1.77
	80	0.471	93.7	2.33
Mean ± Standard deviation	87 ± 12	0.430 ± 0.039	102 ± 7	2.19 ± 0.26
m-Diethylbenzene	80	1.25	144	1.75
	100	0.751	109	1.76
	80	1.16	127	1.73
Mean ± Standard deviation	87 ± 12	1.05 ± 0.27	127 ± 18	1.75 ± 0.02
Malathion	80	1.06	89.4	2.82
	100	0.989	104	1.85
	80	1.70	106	2.07
Mean ± Standard deviation	87 ± 12	1.25 ± 0.39	99.5 ± 8.9	2.25 ± 0.51

Similarly for Recon, the strongest correlations for the averaged data were:

$$P_s = -110\log(t_b) + 210 \quad r = -0.857(p = 3.8 \times 10^{-4}) \tag{7}$$

$$\log(t_b/t_l) = -0.70\log(t_l) + 1.3 \quad r = -0.830(p = 8.2 \times 10^{-4}) \tag{8}$$

$$\log(t_b/t_l) = 0.14D_p - 0.41 \quad r = 0.844(p = 5.6 \times 10^{-4}) \tag{9}$$

$$\log(D_p = -1.0\log(t_l) + 2.3 \quad r = -0.998(p = 2.1 \times 10^{-13}) \tag{10}$$

None of the slopes for the D_p and t_l terms in normal–normal, log–normal, normal–log, and log–log linear relationships differed significantly at $p \leq 0.05$ between Prent and Recon. A similar situation occurred for slopes of t_b/t_l versus t_l, $\log t_l$, and $\log D_p$.

To obtain the most rugged linear correlations between t_l and t_b, the averaged data of Prent and Recon were pooled and correlated again for those slopes showing no significant difference. The pooled regression equations were:

$$t_b/t_l = 0.0050t_l + 1.3 \quad r = -0.955(p = 4.1 \times 10^{-13}) \tag{11}$$

$$t_b/t_l = -1.2\log(t_l) + 3.2 \quad r = -0.921(p = 1.8 \times 10^{-10}) \tag{12}$$

$$t_b/t_l = 0.98\log(D_p) + 0.44 \quad r = 0.879(p = 1.5 \times 10^{-8}) \tag{13}$$

When similar correlation analyses were performed on the individual run data of Prent and Recon respectively, 17 relationships were obtained for Prent and 27 for Recon. Pairing corrects for between-run variations. Slopes showed no significant difference for P_s vs. t_b, $\log P_s$ vs. t_b, and (t_b/t_l) vs. $\log t_l$. On pairing the data for these equations and recorrelating, the significant correlations of the pooled data ($n = 72$) were:

$$P_s = -0.11t_b + 12 \quad r = -0.394(p = 6.2 \times 10^{-4}) \tag{14}$$

$$\log(P_s) = -0.015t_b + 1.5 \quad r = -0.463(p = 4.2 \times 10^{-5}) \tag{15}$$

$$t_b/t_l = -1.3\log(t_l) + 3.5 \quad r = -0.847(p = 6.4 \times 10^{-21}) \tag{16}$$

Eqs. (12) and (16) are very similar and this is probably the most rugged relationship, with the individual run data being of higher statistical power than the average data as expected.

There was no consistent strong relationship between P_s and t_b [Eqs. (3), (7), (14) and (15)]. P_s should be inversely related to $\log t_i$ (where $t_i = t_b$ or t_l) if the chromatographic model applied [9]. However only P_s vs. $\log t_b$ was correlated in Eq. (7). This was also observed for the pure MW 120 alkylbenzene isomers [11].

3.4. Correlation analyses involving permeation kinetic parameters and composition

When the weight percentages (%) of each component were correlated to the permeation characteristics for butyl gloves, no significantly linear correlations were observed at $p \leq 0.05$ for the arithmetic means from Tables 2 and 3, unlike for the individual run

Note to Table 3:
t_b: Breakthrough time; P_s: Steady-state permeation rate; t_l: Lag time; D_p: Diffusion coefficient (calculated from $t_l = l^2/6D_p$); The mean data are expressed in the form of arithmetic mean $\pm$ standard deviation.

Table 4
Correlation analyses of kinetic parameters versus % based on the individual run data of Prent and Recon
(number of observations = 36)

Equation	r
Prent	
$P_s = 3.2\log(\%) + 2.1$	0.514 ($p = 0.0013$)
$\log(P_s) = 0.36\log(\%) + 0.23$	0.50 ($p = 0.0019$)
$P_s / t_1 = 0.055\log(\%) + 0.028$	0.521 ($p = 0.0011$)
$\log(P_s / t_1) = 0.41\log(\%) - 1.7$	0.521 ($p = 0.0011$)
Recon	
$P_s = 3.3\log(\%) + 1.6$	0.490 ($p = 0.0024$)
$\log(P_s) = 0.38\log(\%) + 0.13$	0.522 ($p = 0.0011$)
$P_s / t_1 = 0.038\log(\%) + 0.014$	0.507 ($p = 0.0016$)
$\log(P_s / t_1) = 0.42\log(\%) - 1.9$	0.562 ($p = 3.6 \times 10^{-4}$)

Prent: Prentox™ formulation; Recon: Reconstituted mixture (malathion plus Prentox™ alkylbenzenes); r: Correlation coefficient; p: Probability; P_s: Steady-state permeation rate; t_1: Lag time; %: Weight percentage of each component in Prent and Recon from GC/MS analyses.

data analysis (Table 4). Only the slopes of P_s/t_1 vs. log% were significantly different. On pooling each of the other three homogeneous data sets and recorrelating:

$$P_s = 3.3\log(\%) + 1.8 \quad r = 0.50\left(p = 7.7 \times 10^{-6}\right) \tag{17}$$

$$\log(P_s) = 0.37\log(\%) + 0.18 \quad r = 0.508\left(p = 5.1 \times 10^{-6}\right) \tag{18}$$

$$\log(P_s/t_1) = 0.42\log(\%) - 1.8 \quad r = 0.521\left(p = 2.7 \times 10^{-6}\right) \tag{19}$$

These three linear relationships which involve quantities independent of determination technique will be utilized for further correlation analyses.

3.5. Multiple linear regression analyses

Improved correlations for Eqs. (17)–(19) were examined by adding one of the physical parameters in Table 1 as a second factor (Table 5). No significant correlation contained S_w as a second term. The best models out of the 30 observed were:

$$\log(P_s) = 0.88\log(\%) - 0.0069MW + 0.85 \; r = 0.916\left(p = 4.4 \times 10^{-28}\right) \tag{20}$$

$$\log(P_s/t_1) = 0.96\log(\%) - 0.073MW - 1.1 \; r = 0.891\left(p = 1.8 \times 10^{-24}\right) \tag{21}$$

$$\log(P_s) = 0.83\log(\%) - 9.7\log(d) - 0.53 \; r = 0.919\left(p = 1.5 \times 10^{-28}\right) \tag{22}$$

$$\log(P_s/t_1) = 0.92\log(\%) - 4.4d + 1.9 \; r = 0.897\left(p = 3.8 \times 10^{-25}\right) \tag{23}$$

$$\log(P_s) = 0.87\log(\%) - 0.010MV + 1.4 \; r = 0.902\left(p = 7.9 \times 10^{-26}\right) \tag{24}$$

$$\log(P_s/t_1) = 0.95\log(\%) - 0.011MV - 0.48 \; r = 0.873\left(p = 2.7 \times 10^{-22}\right) \tag{25}$$

$$P_s = 4.2\log(\%) + 4.1\log K_{ow} - 14 \quad r = 0.651 \left(p = 5.4 \times 10^{-9} \right) \tag{26}$$

$$\log(P_s/t_1) = 0.54\log(\%) + 0.52\log K_{ow} - 3.8 \quad r = 0.672 \left(p = 9.8 \times 10^{-10} \right) \tag{27}$$

$$\log(P_s) = 0.41\log(\%) - 0.27\text{DM} + 0.34 \quad r = 0.676 \left(p = 6.9 \times 10^{-10} \right) \tag{28}$$

$$\log(P_s/t_1) = 0.47\log(\%) - 0.30\text{DM} - 1.6 \quad r = 0.691 \left(p = 1.8 \times 10^{-10} \right) \tag{29}$$

$$P_s = 4.2\log(\%) - 70E^o + 17 \quad r = 0.651 \left(p = 5.4 \times 10^{-9} \right) \tag{30}$$

$$\log(P_s/t_1) = 0.54\log(\%) - 8.8E^o + 0.18 \quad r = 0.672 \left(p = 9.8 \times 10^{-10} \right) \tag{31}$$

Comparable relationships were found for the same solutions challenging nitrile gloves [8]. However, the slopes and intercepts differed, reflecting interactions with different glove types. As for nitrile, p-values are lowest for regressions involving MW, d, and MV relative to $\log K_{ow}$, DM and E^o. MV did not show the lowest p-value unlike for nitrile. Each second term for butyl gloves makes larger contributions than for nitrile.

   Based on Table 5, correlation analyses were redone by adding another physical parameter from Table 1 as a third term. Thirty-five significant relationships resulted. The equations with highest power contain logMV as second term, or $\log K_{ow}$, DM and $\log E^o$ as third term:

$$\log(P_s) = 0.89\log(\%) - 4.1\log(\text{MV}) + 0.28\log K_{ow} + 7.7$$
$$r = 0.919 \left(p = 1.8 \times 10^{-27} \right) \tag{32}$$

$$\log(P_s/t_1) = 0.97\log(\%) - 4.1\log(\text{MV}) + 0.36\log K_{ow} + 5.5$$
$$r = 0.899 \left(p = 2.2 \times 10^{-24} \right) \tag{33}$$

$$\log(P_s) = 0.83\log(\%) - 4.0\log(\text{MV}) - 0.098\text{DM} + 8.6$$
$$r = 0.897 \left(p = 4.0 \times 10^{-24} \right) \tag{34}$$

$$\log(P_s/t_1) = 0.88\log(\%) - 4.0\log(\text{MV}) - 0.13\text{DM} + 6.6$$
$$r = 0.871 \left(p = 6.4 \times 10^{-21} \right) \tag{35}$$

$$\log(P_s) = 0.90\log(\%) - 4.2\log(\text{MV}) - 2.5\log(E^o) + 7.3$$
$$r = 0.921 \left(p = 7.0 \times 10^{-28} \right) \tag{36}$$

$$\log(P_s/t_1) = 0.98\log(\%) - 4.3\log(\text{MV}) - 3.2\log(E^o) + 5.0$$
$$r = 0.901 \left(p = 1.3 \times 10^{-24} \right) \tag{37}$$

Eq. (32) is probably the best equation to use for further model building since the p-value of Eq. (36) though lower is derived indirectly from the calculated relationship of $\log K_{ow}$ and E^o. Addition of a fourth term from Table 1 did not improve p further.

   When calculated $\log P_s$ and observed $\log P_s$ were linearly regressed for Eq. (32), the slope was 1.00 and 1,2,3-trimethylbenzene was the compound most away from the mean line. The same results occurred for Eq. (33) though 1,2,3-trimethylbenzene was closer to the mean line. Comparable models were also applicable for permeation through nitrile. The corresponding slopes of log% are significantly different at $p \leq 0.05$ for nitrile and

Table 5
Significant correlations at $p \leq 0.05$ of permeation kinetic parameters versus % and physical parameters from Table 1 based on the pooled individual run data of Prent and Recon (number of observations = 72)

Equation	r
$P_s = 7.6\log(\%) - 0.058\text{MW} + 7.5$	$0.873\ (p = 2.9 \times 10^{-22})$
$\log(P_s) = 0.88\log(\%) - 0.0069\text{MW} + 0.85$	$0.916\ (p = 4.4 \times 10^{-28})$
$P_s = 7.5\log(\%) - 27\log(\text{MW}) + 56$	$0.864\ (p = 2.4 \times 10^{-21})$
$\log(P_s) = 0.88\log(\%) - 3.2\log(\text{MW}) + 6.7$	$0.913\ (p = 1.2 \times 10^{-27})$
$\log(P_s / t_1) = 0.96\log(\%) - 0.0073\text{MW} - 1.1$	$0.891\ (p = 1.8 \times 10^{-24})$
$\log(P_s / t_1) = 0.95\log(\%) - 3.3\log(\text{MW}) + 5.0$	$0.882\ (p = 3.1 \times 10^{-23})$
$P_s = 7.1\log(\%) - 34d + 30$	$0.853\ (p = 3.3 \times 10^{-20})$
$\log(P_s) = 0.83\log(\%) - 4.1d + 3.7$	$0.918\ (p = 1.8 \times 10^{-28})$
$P_s = 7.0\log(\%) - 78\log(d) - 3.9$	$0.848\ (p = 8.5 \times 10^{-20})$
$\log(P_s) = 0.83\log(\%) - 9.7\log(d) - 0.53$	$0.919\ (p = 1.5 \times 10^{-28})$
$\log(P_s / t_1) = 0.92\log(\%) - 4.4d + 1.9$	$0.897\ (p = 3.8 \times 10^{-25})$
$\log(P_s / t_1) = 0.91\log(\%) - 10\log(d) - 2.5$	$0.896\ (p = 4.6 \times 10^{-25})$
$P_s = 7.6\log(\%) - 0.087\text{MV} + 13$	$0.866\ (p = 1.9 \times 10^{-21})$
$\log(P_s) = 0.87\log(\%) - 0.010\text{MV} + 1.4$	$0.902\ (p = 7.9 \times 10^{-26})$
$P_s = 7.4\log(\%) - 37\log(\text{MV}) + 80$	$0.849\ (p = 8.1 \times 10^{-20})$
$\log(P_s) = 0.86\log(\%) - 4.4\log(\text{MV}) + 9.4$	$0.885\ (p = 1.1 \times 10^{-23})$
$\log(P_s / t_1) = 0.95\log(\%) - 0.011\text{MV} - 0.48$	$0.873\ (p = 2.7 \times 10^{-22})$
$\log(P_s / t_1) = 0.93\log(\%) - 4.6\log(\text{MV}) + 7.8$	$0.852\ (p = 4.3 \times 10^{-20})$
$P_s = 4.2\log(\%) + 4.1\log K_{\text{ow}} - 14$	$0.651\ (p = 5.4 \times 10^{-9})$
$\log(P_s) = 0.47\log(\%) + 0.43\log K_{\text{ow}} - 1.5$	$0.644\ (p = 9.6 \times 10^{-9})$
$\log(P_s / t_1) = 0.54\log(\%) + 0.52\log K_{\text{ow}} - 3.8$	$0.672\ (p = 9.8 \times 10^{-10})$
$P_s = 3.6\log(\%) - 2.3\text{DM} + 3.2$	$0.652\ (p = 5.0 \times 10^{-9})$
$\log(P_s) = 0.41\log(\%) - 0.27\text{DM} + 0.34$	$0.676\ (p = 6.9 \times 10^{-10})$
$\log(P_s / t_1) = 0.47\log(\%) - 0.30\text{DM} - 1.6$	$0.691\ (p = 1.8 \times 10^{-10})$
$P_s = 4.2\log(\%) - 70E^o + 17$	$0.651\ (p = 5.4 \times 10^{-9})$
$\log(P_s) = 0.47\log(\%) - 7.4E^o + 1.8$	$0.644\ (p = 9.6 \times 10^{-9})$
$P_s = 4.1\log(\%) - 34\log(E^o) - 20$	$0.631\ (p = 2.5 \times 10^{-8})$
$\log(P_s) = 0.46\log(\%) - 3.6\log(\text{E}^o) - 2.1$	$0.624\ (p = 4.0 \times 10^{-8})$
$\log(P_s / t_1) = 0.54\log(\%) - 8.8E^o + 0.18$	$0.672\ (p = 9.8 \times 10^{-10})$
$\log(P_s / t_1) = 0.53\log(\%) - 4.3\log(E^o) - 4.6$	$0.652\ (p = 5.0 \times 10^{-9})$

r: Correlation coefficient; p: Probability; P_s: Steady-state permeation rate; t_1: Lag time; %: Weight percentage of each component in Prent and Recon; MW: Molecular weight; d: Liquid density at 20°C; MV: Molar volume at 20°C; $\log K_{\text{ow}}$: The logarithm to base 10 of the octanol/water partition coefficient at 25°C; DM: Dipole moment of the liquid at 20–30°C in Debye; E^o: Calculated Snyder elution strength.

butyl materials. Again, the slopes for the second and third terms are larger for butyl than nitrile. As for nitrile gloves, Eqs. (32)–(37) constitute predictive equations reflecting the interaction between the challenge solution and the glove material that correct for mixture composition, molar volume and partitioning/hydrophobicity.

3.6. Correlation analyses between kinetic parameters and the physical properties of the chemicals without accounting for composition

The physical parameters of Table 1 were also correlated to the permeation kinetic parameters independent of % but no significant correlations at $p \leq 0.05$ were found for

the averaged data of Prent and Recon. Twenty-six correlations for $p \leq 0.05$ were found for the individual run data of Prent ($n = 36$). The strongest correlations were:

$$\log(P_s) = -0.27DM + 0.60 \quad r = -0.468 \ (p = 0.0040) \tag{38}$$

$$\log(P_s/t_1) = -0.33DM - 1.2 \quad r = -0.504 \ (p = 0.0017) \tag{39}$$

$$\log(P_s/t_1) = -7.0E^o + 0.15 \quad r = -0.362 \ (p = 0.030) \tag{40}$$

$$D_p = -12E^o + 6.4 \quad r = -0.342 \ (p = 0.041) \tag{41}$$

For Recon at $p \leq 0.05$ and $n = 36$, only $\log S_w$ vs. $\log t_1$ was significant:

$$\log(t_1) = -0.038\log(S_w) + 2.1 \quad r = -0.366 \ (p = 0.028) \tag{42}$$

This is the only relationship involving S_w for both nitrile and butyl for Prent and Recon challenges. The correlation of $\log S_w$ and $\log K_{ow}$, at $p \leq 0.05$, $n = 12$ (Table 1) was:

$$\log(S_w) = -1.2\log K_{ow} + 6.0 \quad r = -0.785 \ (p = 0.0025) \tag{43}$$

Compare

$$\log(S_w) = -1.3\log K_{ow} + 6.0 \tag{44}$$

from ref. 13, a well known correlation that shows acceptable agreement. Yet $\log K_{ow}$ did not correlate to $\log t_1$ in spite of Eqs. (42) and (43). Thus, no comparable correlations were observed between Prent and Recon. The term % must be included.

3.7. Retention volume analyses

Table 6 shows the retention volumes ($V_R(t_1)$ and $V_R(t_{s1})$) of each component in Prent and Recon where the first observed time in the steady-state period is denoted as t_{s1} [8]. Only the $V_R(t_1)$ and $V_R(t_{s1})$ for mesitylene, 1,2,4-trimethylbenzene, and 1,2,3-trimethylbenzene were significantly different at $p \leq 0.05$. For Prent, only the $V_R(t_1)$ and $V_R(t_{s1})$ of m-xylene differed and for Recon, those of mesitylene and 1,2,3-trimethylbenzene. In contrast, for the nitrile-butyl glove comparison all $V_R(t_1)$ and $V_R(t_{s1})$ values for Prent were lower for butyl than nitrile. This implies that nitrile can actually hold more formulation than butyl. Since the butyl gloves had an average thickness of 0.39 ± 0.02 mm and nitrile gloves was of 0.62 ± 0.02 mm thickness, this agrees with expectation.

Correlation analyses between $V_R(t_1)$ and $V_R(t_{s1})$ and % showed significant linear relationships at $p \leq 0.05$ ($n = 36$) for Prent:

$$V_R(t_1) = 0.00076\log(\%) + 0.00098 \quad r = 0.361 \ (p = 0.031) \tag{45}$$

$$\log(V_R(t_1)) = 0.25\log(\%) - 3.2 \quad r = 0.329 \ (p = 0.050) \tag{46}$$

$$\log(V_R(t_{s1})) = 0.27\log(\%) - 3.1 \quad r = 0.340 \ (p = 0.043) \tag{47}$$

For Recon, the same correlations were found at greater significance:

$$V_R(t_1) = 0.0014\log(\%) + 0.00092 \quad r = 0.441 \ (p = 0.0071) \tag{48}$$

$$\log(V_R(t_1)) = 0.28\log(\%) - 3.1 \quad r = 0.385 \ (p = 0.020) \tag{49}$$

$$\log(V_R(t_{s1})) = 0.29\log(\%) - 3.1 \quad r = 0.396 \ (p = 0.017) \tag{50}$$

Table 6
Averaged retention volumes for Prent and Recon challenges through unlined unsupported butyl gloves

Compound	$V_R(t_1)$		$V_R(t_{s1})$	
	Prent	Recon	Prent	Recon
m-Xylene	0.00270	0.00161	0.00404	0.00174
	(0.00056)	(0.00053)	(0.00050)	(0.00046)
o-Xylene	0.000447	0.000711	0.000510	0.000749
	(0.000086)	(0.000214)	(0.000141)	(0.000230)
Cumene	0.000591	0.00126	0.000650	0.00154
	(0.000038)	(0.00040)	(0.000043)	(0.00062)
n-Propylbenzene	0.00115	0.00139	0.00120	0.00147
	(0.00045)	(0.00032)	(0.00040)	(0.00028)
3-Ethyltoluene	0.00339	0.00375	0.00366	0.00483
	(0.00070)	(0.00058)	(0.00095)	(0.00052)
4-Ethyltoluene	0.00182	0.00151	0.00212	0.00154
	(0.00095)	(0.00009)	(0.00053)	(0.00003)
Mesitylene	0.00141	0.000588	0.00167	0.000669
	(0.00021)	(0.000025)	(0.00029)	(0.000011)
2-Ethyltoluene	0.000806	0.00118	0.00112	0.00127
	(0.000306)	(0.00035)	(0.00025)	(0.00045)
1,2,4-Trimethylbenzene	0.00308	0.00618	0.00365	0.00651
	(0.00028)	(0.00085)	(0.00034)	(0.00084)
1,2,3-Trimethylbenzene	0.000163	0.000211	0.00017	0.000235
	(0.000021)	(0.000004)	(0.00002)	(0.000011)
m-Diethylbenzene	0.000597	0.000689	0.000627	0.000804
	(0.000089)	(0.000253)	(0.000124)	(0.000341)
Malathion	0.000365	0.000442	0.000438	0.000502
	(0.000181)	(0.000166)	(0.000183)	(0.000187)

Prent: Data of Prentox™ formulations for material of 0.39 ± 0.02 mm thickness; Recon: Data of reconstitution mixtures for material of 0.36 ± 0.02 mm thickness; $V_R(t_1)$: Retention volume in ml [calculated based on the lag time (t_1)]; $V_R(t_{s1})$: Retention volume in ml [calculated based on the first time point of the steady-state period (t_{s1})]; The averaged data are expressed in the form of arithmetic mean (standard deviation).

The corresponding slopes of Eqs. (46) and (47) did not significantly differ from those of Eqs. (49) and (50) at $p \leq 0.05$. On data pooling and recorrelating ($n = 72$):

$$\log(V_R(t_1)) = 0.27\log(\%) - 3.1 \quad r = 0.355 \,(\, p = 0.0022) \tag{51}$$

$$\log(V_R(t_{s1})) = 0.28\log(\%) - 3.1 \quad r = 0.366 \,(\, p = 0.015) \tag{52}$$

The correlation between $\log V_R(t_{s1})$ and log% was also observed in the permeation study of nitrile gloves [8]. However for $V_R(t_1)$, the strongest relationship was the normal–log correlation for nitrile gloves [8].

The physical parameters from Table 1 were added to Eqs. (51) and (52) as a second term for further analyses. Table 7 shows the twenty significant relationships at $p \leq 0.05$ ($n = 72$). The corresponding relationships for $\log V_R(t_1)$ are more powerful than for $\log V_R(t_{s1})$. Also, the log–log correlation is more statistically sensitive than the log–normal correlation for the same set of variables. MW, d, or MV as second terms were superior to $\log K_{ow}$, DM or E^o.

Table 7
Correlation analyses of retention volumes versus log% and physical parameters from Table 1 for butyl gloves (number of observations = 72)

Equation	r
$\log(V_R(t_1)) = 0.80\log(\%) - 0.0072\text{MW} - 2.4$	$0.849\ (p = 7.3 \times 10^{-20})$
$\log(V_R(t_1)) = 0.80\log(\%) - 3.4\log(\text{MW}) + 3.7$	$0.850\ (p = 6.7 \times 10^{-20})$
$\log(V_R(t_{s1})) = 0.82\log(\%) - 0.0072\text{MW} - 2.4$	$0.847\ (p = 1.2 \times 10^{-19})$
$\log(V_R(t_{s1})) = 0.82\log(\%) - 3.4\log(\text{MW}) + 3.9$	$0.849\ (p = 7.4 \times 10^{-20})$
$\log(V_R(t_1)) = 0.76\log(\%) - 4.3d + 0.50$	$0.848\ (p = 9.5 \times 10^{-20})$
$\log(V_R(t_1)) = 0.75\log(\%) - 10\log(d) - 3.9$	$0.850\ (p = 6.2 \times 10^{-20})$
$\log(V_R(t_{s1})) = 0.78\log(\%) - 4.4d + 0.57$	$0.843\ (p = 2.8 \times 10^{-19})$
$\log(V_R(t_{s1})) = 0.77\log(\%) - 10\log(d) - 3.8$	$0.845\ (p = 1.8 \times 10^{-19})$
$\log(V_R(t_1)) = 0.80\log(\%) - 0.011\text{MV} - 1.8$	$0.833\ (p = 1.9 \times 10^{-18})$
$\log(V_R(t_1)) = 0.79\log(\%) - 4.7\log(\text{MV}) + 6.7$	$0.821\ (p = 1.7 \times 10^{-17})$
$\log(V_R(t_{s1})) = 0.82\log(\%) - 0.011\text{MV} - 1.8$	$0.832\ (p = 2.1 \times 10^{-18})$
$\log(V_R(t_{s1})) = 0.81\log(\%) - 4.7\log(\text{MV}) + 6.9$	$0.823\ (p = 1.2 \times 10^{-17})$
$\log(V_R(t_1)) = 0.36\log(\%) + 0.40\log K_{ow} - 4.7$	$0.503\ (p = 4.2 \times 10^{-5})$
$\log(V_R(t_{s1})) = 0.37\log(\%) + 0.38\log K_{ow} - 4.5$	$0.495\ (p = 6.1 \times 10^{-5})$
$\log(V_R(t_1)) = 0.31\log(\%) - 0.27\text{DM} - 3.0$	$0.560\ (p = 2.4 \times 10^{-6})$
$\log(V_R(t_{s1})) = 0.32\log(\%) - 0.27\text{DM} - 2.9$	$0.558\ (p = 2.5 \times 10^{-6})$
$\log(V_R(t_1)) = 0.36\log(\%) - 6.9E^o - 1.6$	$0.499\ (p = 5.1 \times 10^{-5})$
$\log(V_R(t_1)) = 0.34\log(\%) - 3.3\log(E^o) - 5.3$	$0.477\ (p = 1.4 \times 10^{-4})$
$\log(V_R(t_{s1})) = 0.37\log(\%) - 6.5E^o - 1.6$	$0.491\ (p = 7.4 \times 10^{-5})$
$\log(V_R(t_{s1})) = 0.36\log(\%) - 3.1\log(E^o) - 5.1$	$0.470\ (p = 1.8 \times 10^{-4})$

r: Correlation coefficient; p: Probability; $V_R(t_1)$: Retention volume [calculated based on the lag time (t_1)]; $V_R(t_{s1})$: Retention volume [calculated based on the first time point of the steady-state period (t_{s1})]; %: Weight percentage of each component in Prent and Recon from GC/MS analyses; MW: Molecular weight; d: Liquid density at 20°C; MV: Molar volume at 20°C; $\log K_{ow}$: The logarithm to base 10 of the octanol/water partition coefficient at 25°C; DM: Dipole moment of the liquid at 20–30°C in Debye; E^o: Calculated Snyder elution strength.

Again adopting a log% first term and a logMV or logMW or $\log d$ second term, a third physical parameter was tested for improvement in p. Eight relationships were found with high r and low p-values. Comparable models for $V_R(t_{s1})$ were also observed in the nitrile study [8]. Due to their low p-values and the similar models shown for nitrile, the best models were selected as:

$$\log(V_R(t_{s1})) = 0.83\log(\%) - 4.5\log(\text{MV}) - 0.21\log K_{ow} + 5.6$$

$$r = 0.848\ (p = 1.1 \times 10^{-18}) \tag{53}$$

$$\log(V_R(t_{s1})) = 0.84\log(\%) - 4.5\log(\text{MV}) - 0.20\log(E^o) + 5.1$$

$$r = 0.846\ (p = 1.7 \times 10^{-18}) \tag{54}$$

Compared with the corresponding relationships for nitrile gloves [8], the regression weights for nitrile are larger than for butyl for log%, the third term, and the intercept but not for logMV. This indicates that different glove materials affect these equations. Addition of further terms from Table 1 did not improve p.

4. Conclusions

Correlations among P_s, log%, and MW, $\log d$, MV, $\log K_{ow}$ or DM were established for butyl gloves when challenged with the same malathion formulation and the reconstituted cocktail of malathion and alkylbenzene inert components. The contributions of composition and molar volume must be factored out before hydrophobicity becomes significant. The generality of the predictive equations should be tested with other formulations and gloves.

Acknowledgements

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