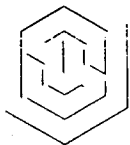


DEPARTMENT OF
BIORESOURCE
ENGINEERING

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Dr. D. Keith Cassel
Editor, SSSA Journal
Department of Soil Science
North Carolina State University
P.O. Box 7619
Raleigh, NC 27695-7619



OREGON
STATE
UNIVERSITY

Gilmore Hall 116
Corvallis, Oregon
97331-3906

Dear Dr. Cassel,

Please find four copies of the manuscript "Analysis of Disperse Dyes and FD&C Blue No. 1 as Tracers for Pesticides" for consideration for publication in the Soil Science Society of America Journal, S-1 Division. I will be the corresponding author for this publication which was jointly prepared by R.A. Pangia, J. E. Baham and myself. As always, you or any other Journal editors should feel free to contact me at any time if there are any questions.

Sincerely,

A handwritten signature in black ink, appearing to read 'John S. Selker'.

John S. Selker
rm 240 Gilmore Hall
Oregon State University
Corvallis, OR 97331-3906
phone: 541-737-6304
FAX: 541-737-2082
email: selkerj@ccmail.orst.edu

cc. R.A. Pangia
J.E. Baham
W. Crannell

Telephone
Departmental
503-737-2041

Extension
503-737-4021

Fax
503-737-2082

1 **Analysis of Disperse Dyes and FD&C Blue No. 1**

2 **as Tracers for Pesticides**

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4 **Ruth A. Pangia, John S. Selker and John E. Baham**

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8 submitted to

9 Soil Science Society of America Journal

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16 Pangia, Ruth A., John S. Selker *, and John E. Baham

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18 R. A. Pangia and J. S. Selker, Dept. of Bioresource Engineering, and J. E. Baham, Dept.
19 of Crops and Soil Science, Oregon State University, Corvallis, Oregon, 97331.

20 * Corresponding author.

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1 **Analysis of Disperse Dyes and FD&C Blue No. 1**
2 **as Tracers for Pesticides**

3
4 **ABSTRACT**

5
6 Contamination of water sources due to the use of agricultural chemicals can be
7 minimized through understanding the transport relationships for organic chemicals in soil
8 environments. In this study we evaluated seven non-hazardous dyes that have properties
9 which were consistent with application as surrogates to organic agro-chemicals to assess
10 mobility through soils with respect to adsorption and desorption mechanisms. This study
11 presents the batch adsorption method to obtain soil/water partition coefficients (K_d) for
12 both adsorption and desorption experiments and octanol/water partition coefficients (K_{ow}).
13 Six hydrophobic disperse dyes were examined and one hydrophilic Food, Dye & Colorant
14 Blue No. 1. Parameter testing of pH stability and adsorption ratios eliminated five dyes;
15 Disperse Violet No. 1 and FD&C Blue No. 1 remained to be examined in detail. Two
16 soil minerals were employed to demonstrate sorption properties of the dyes; a soil sample
17 from the B horizon of a Woodburn silt loam and a 30/40 grade clean silica sand.
18 Significant hysteresis was observed between adsorption and desorption processes for the
19 two dyes in the Woodburn soil, suggesting that these dyes do not have fully reversible
20 desorption characteristics when organic matter and the Cation Exchange Capacity (CEC)
21 play a role in organic chemical mobility. Our soil/water batch experiments show that
22 FD&C Blue Dye No. 1 is suitable for use as a tracer for hydrophilic agro-chemicals that

1 have potential to leach through the soil. Disperse Violet No. 1 was found to be an
2 acceptable tracer for laboratory studies to examine the mobility of hydrophobic agro-
3 chemicals that are similarly adsorbed. Experimental K_{ow} values corresponded directly to
4 the prediction of dye partitioning; 7.0×10^{-03} for FD&C Blue No. 1 suggested no
5 partitioning into organic matter, where $6.3 \times 10^{+05}$ for Disperse Violet No.1 suggested
6 strong partitioning into organic matter.

7

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INTRODUCTION

9

10 Issues tied to the increased use of agricultural chemicals are accumulation of
11 chemical residues in soil and leaching of residues into water supplies. A number of
12 midwestern states have found potentially harmful organic compounds in wells and
13 reservoirs to be at levels outside of the standards suggested by the U.S. Environmental
14 Protection Agency (Agertved, 1992). The standards with which agricultural chemicals
15 are being applied are being questioned and the registration of many commonly used
16 agricultural chemicals are being re-evaluated at this time.

17 Unique characteristics of each chemical and soil type can create potentially
18 hazardous leaching and accumulation conditions which are difficult to predict. Processes
19 affecting the mobility and fate of organic chemicals through soil include: adsorption and
20 desorption by soil organic matter or mineral surfaces, biodegradation and volatilization
21 (Kerle et al., 1993; Trudgill, 1987). It has been suggested, however, that the likelihood
22 of leaching can be related in broad terms to the soil texture, pH and organic matter

1 content (USEPA, 1988). At present the only accurate means of verifying a chemical's
2 activity in a specific soil is to apply it to a crop and trace it's movement, often requiring
3 the use of radioactively labeled compounds. As well as being expensive, radioactive
4 tagging is strictly regulated by the federal government (Davis et al., 1980), and is thus not
5 practically applicable to most sites. Taken together the now difficult task of tracking
6 pesticide movement and our inability to reliably predict transport, a tracer which
7 reproduces pesticide transport properties and is inexpensive to assay for would greatly
8 expand our ability to predict movement under field conditions. Colored tracers appear to
9 be excellent candidates for this application due to their wide range of chemical properties
10 and low cost analysis opportunities (Butters and Bandaranayake, 1993a).

11 Fluorescent and non-fluorescent dyes have long been employed as hydrologic tracers.
12 Smart and Laidlaw (1977) provided a seminal work based upon an extensive review of
13 sediment batch experiments, and soil column studies to analyze the mobility and stability of
14 eight of the most commonly used fluorescent dyes in hydrology. Smettem and Trudgill (1983)
15 documented breakthrough curves for several of these same fluorescent and non-fluorescent
16 tracers in a well characterized soil. Ionic activity, adsorption and chemical decay properties of
17 the tracers were considered in their study. Sabatini and Austin (1991) investigated the
18 utility of non-hazardous rhodamine WT and fluorescein as adsorbing tracers for
19 agricultural chemicals in soils. Their study showed that fluorescent dyes have erratic
20 adsorption patterns and, therefore, may not be useful as tracers. Baughman and Perenich
21 (1988) stimulated interest in hydrophobic disperse dyes used for dyeing fabrics. They implied
22 that these dyes adsorb to sediments in the same manner as hydrophobic pollutants, suggesting

1 that these dyes may have predictable movements through soil comparable to agricultural
2 chemicals. Following on the work of Andreini and Steenhuis (1990), Flury and Fluhler
3 (1994) examined the suitability of FD&C Blue Dye No. 1 as a hydrophilic dye tracer from
4 a toxicological perspective, with a follow up article (Flury and Fluhler, 1995) considering
5 the equilibrium partitioning coefficients in three soils. Butters and Bandaranayake
6 (1993a) created a class room demonstration using FD&C Blue Dye No. 1 to show the
7 transport system in relation to the chemistry of the dyes and the properties of the soil.

8 This research examines six hydrophobic disperse dyes discussed by Baughman and
9 Perenich (1988) as well as the hydrophilic dye FD&C Blue Dye No. 1 (Table 1). The
10 following properties were assessed in order to determine predictable reactions in soil:

- 11 (1) adsorption to soil from aqueous solution, K_{da} ;
- 12 (2) desorption from the soil to aqueous solution, K_{dd} ;
- 13 (3) and, partitioning of the dyes between octanol and water, K_{ow} .

14 Retardation factors (R), and partitioning relating to organic carbon content of the soil (K_{oc})
15 were also calculated to illustrate potential movement of the dyes in soil. These experimental
16 partitioning coefficients and calculated values provide information about the distribution of the
17 dyes in soil which may be compared to a range of known experimental coefficients for
18 agricultural chemicals derived by the USEPA. These comparisons will allow the selection of
19 suitable dyes to use as tracers for given compounds that can be assessed in a variety of
20 soils without presenting their own inherent hazardous effects.

21

22

TRACER SELECTION CRITERIA

1
2
3 There are several issues which must be considered when selecting dyes to mimic
4 contaminant mobility in soil. A tracer must be inexpensive both in application and assay;
5 non-toxic; have a useful half-life; be chemically stable, and have an absorption maxima
6 between 400 and 650 nm (Gasper, 1987; Trudgill, 1987). A tracer must also be easily
7 detected at low concentrations and not modify the natural movement of water (Davis et
8 al., 1980). Non-fluorescent dyes are preferable to fluorescent dyes due to the simple and
9 inexpensive methods of assay, and on the basis of the Sabatini and Austin (1991)
10 investigation, this study is restricted to non-fluorescent dyes.

11 Dyes generally travel slower than single atom anions through soil due to their potential
12 to react with negatively charged mineral surfaces and their affinity to adsorb to organic matter.
13 In order to assess the differences in characteristic adsorption and desorption processes both
14 hydrophobic and hydrophilic dyes were chosen for this analysis. In order to eliminate strong
15 cation exchange effects inherent in the soil, the dyes chosen are anions in $\text{pH} > 8$ and neutral at
16 $\text{pH} < 6$. These characteristics imply that these dyes will pass through soil media with the water
17 at high pH due to their anionic nature, and that there will be some retardation at lower pH due
18 to their neutral nature creating temporary bonding with organic matter and the soil mineral
19 surfaces. At any pH, however, organic matter will play a prominent role in the mobility of the
20 hydrophobic dyes due to their natural affinity to the hydrophobic regions of organic material
21 (Ware, 1992).

MATERIALS AND METHODS

Parameter Testing

Stock solutions for the hydrophobic disperse dyes at their solubility limit were prepared by dissolving the dye at 25 C° in 0.01 M CaCl₂. After 24 hours the aqueous dyes were filtered several times through borosilicate filter paper. Two experiments were performed to eliminate those dyes which did not satisfy the parameters described below. The first set of experiments was designed to determine the effect of phase or chemical changes correlated with changes of pH in the system on the solutions solubility and adsorption maxima. All of the dyes were mixed in buffered solutions of pH 4, 7, and 10.

The second set of experiments were performed in order to determine the optimal ratio of soil to dye solution. Constant concentrations of dye solution were mixed with the soils whose masses varied from 0.05 to 15 g. The solutions were shaken for 6 hours and the supernatant was pipetted off and analyzed with a spectrophotometer. Graphs were developed relating the mass of the soil verses the concentration of the dye remaining in solution after adsorption. The soil mass that displayed an adequate concentration\soil ratio was chosen for the batch adsorption studies later (Green et al., 1980).

These screening procedures reduced the candidate dyes to two: the hydrophobic dye Disperse Violet No. 1, and the hydrophilic dye FD&C Blue No. 1 (Figures 1 and 2). Since these two dyes were not purified before analysis, their molar absorbtivity coefficients (ϵ_{λ} , L mol⁻¹ cm⁻¹) of Beer's Law ($A=\epsilon_{\lambda}bc$), were determined. Seven dye/water solutions with varying concentrations were prepared and analyzed using a spectrophotometer.

1

2 **Batch Study for Soil Partitioning**

3 This study assesses the dyes potential for adsorption and desorption when dissolved in
4 solutions of pH 4 and 8 at a constant temperature of 25 C°. Variables were: (1) dye
5 concentration and (2) soil type (Table 2). The dye concentrations ranged from 26 to 1.0 (μmol
6 L^{-1}) for the FD&C Blue dye, and 2.0 to 0.1 (pmol L^{-1}) for the Disperse Violet dye. The
7 Woodburn soil series was obtained from a Willamette Valley site, at a depth of 0 cm to 75 cm.
8 This soil was air dried, sieved and blended into a homogenous media of particles ≤ 2 mm.
9 The clean silica sand, trade name "Accusand®"¹ was purchased from Unimin Corp., Le
10 Sueur, MN, presieved to a 30/40 grade. All experiments were performed in silica test
11 tubes with standard septum caps. In order to minimize loss of dye onto the caps, they
12 were separated from the supernatant with a standard elastic laboratory film.

13 Approximately 5.0 g of Woodburn soil, or 15.0 g of Accusand, was mixed with 25
14 mL of aqueous dye solution at varying concentrations. Adsorption kinetic studies
15 demonstrated that 6 hours of reaction time was needed to reach equilibrium. After 6 hours of
16 shaking a 24 hour period was allowed for settling. The Woodburn supernatant was
17 centrifuged at 5000 g-force for 15 minutes to remove suspended soil sediments. Ten
18 milliliters of supernatant was pipetted from the centrifuge tube and the concentration of

¹ Reference to trade names or companies is made for information purposes only and does not imply endorsement by Oregon State University.

1

2 dye remaining in solution after adsorption was determined. Desorption experiments were
3 run immediately after the adsorption experiments. Ten milliliters of 0.01 M CaCl₂
4 solution was returned to each of the test tubes. These were shaken for 6 hours and then
5 allowed to settle for 24 hours to return to equilibrium. The extraction and shaking
6 procedure was repeated twice before spectral analysis.

7 In order to determine concentrations that were adsorbed and desorbed from the
8 soils the supernatant was analyzed in quartz cuvetts with a Beckman UV/VIS
9 spectrophotometer, model DU-62; 625 and 553 nm for FD&C Blue No. 1 and Disperse
10 Violet No. 1 respectively. The amount of dye sorbed was determined as the difference
11 between the total amount added and that remaining in solution after 6 hours of reaction
12 time.

13

14 **Batch Study for Octanol/Water Partitioning**

15 The octanol/water partition coefficients (K_{ow}), were determined using *n*-octanol and
16 distilled water (USEPA, 1975). The partitioning experiment used 15 mL of 99.3% pure
17 *n*-octanol at equilibrium with 15 mL distilled water in the same glass tubes and caps
18 described above. Six different concentrations of dye were assessed: 1.0×10^{-7} to $4.2 \times$
19 10^{-6} (mol L⁻¹) for FD&C Blue No. 1 and 8.4×10^{-5} to 4.5×10^{-4} (mol L⁻¹) for Disperse
20 Violet No. 1 were used, with four replicates of each. After the octanol/water system was
21 shaken and allowed to come to equilibrium, the dye was added as a solid. The system
22 was shaken again at a constant temperature of 25 C° for 3 hours and was then allowed to

1 settle for 24 hours in order to achieve equilibrium. Both dye systems were centrifuged at
2 2500 g-force for 30 minutes in order to minimize the emulsion phase between the octanol
3 and water phases. The concentration of dye in the aqueous and the organic phases was
4 analyzed spectroscopically as described above.

5

6

RESULTS AND DISCUSSION

7

8 Suitability Screening

9 Solvent Blue #59 was eliminated at due to it's extreme insolubility. Disperse dyes
10 Violet No. 8 and Blue No. 23 and 79 displayed pronounced bathachromic shifts and were
11 excluded from further consideration. Disperse Blue Dye No. 3 displayed erratic adsorption
12 behavior during the soil/dye ratio studies and was also excluded from the rest of the
13 experiments.

14

15 Adsorption and Desorption

16 Distinct differences in the adsorption and desorption of the two dyes to the
17 Woodburn silt loam and the Accusand were determined (Table 3) and can be attributed to
18 the differences in organic matter and the CEC of the two media. Mingelgrin and Gerstl
19 (1983) found a correlation between partitioning of organic compounds from aqueous
20 solution to soils to be controlled by the organic carbon content which can then be directly
21 related to the octanol water partition coefficient, (K_{ow}). Our results show that the
22 adsorption and desorption coefficients for the hydrophobic Disperse Violet No. 1 in the

1 Woodburn soil are consistently several orders of magnitude greater than those in the
2 Accusand. Since Accusand contains less than 0.03% organic matter (Schroth et al.,
3 1995), it can be assumed that organic matter is a dominant mechanism for adsorption in
4 the Woodburn soil. The experimentally high K_{ow} of the Disperse Violet No. 1 also
5 supports this assumption due to the affinity for this dye to partition into organic matter.

6 Yen et al. (1991) suggests absorption patterns for Disperse Violet No. 1 are
7 related to the CEC of the soil. Our study supports the observation that the CEC and the
8 organic matter content of a soil system contributes to the mechanistic forces for the
9 adsorption and desorption of the hydrophobic Disperse Violet. In the Accusand at pH 8
10 it was determined that the adsorption of the Disperse Violet was 57% greater than at pH
11 4. This suggests that the silanol groups at pH 4 are partially protonated, and are thereby
12 inhibiting sorption of the dye. The Woodburn soil, in contrast, was found to have 66%
13 less adsorption at pH 8 than at pH 4. This suggests that at pH 8 the Woodburn soil
14 maintains its negative charge and since Disperse Violet is an anion, there is less
15 adsorption. Changing the pH of the dye solution has a large effect on the Disperse Violet
16 molecule and therefore, at pH 4 the dye and portions of the soil are protonated, allowing
17 the CEC of the soil system to take effect. The experimental K_d 's in the Woodburn soil
18 and K_{ow} for Disperse Violet are magnitudes greater than those of FD&C Blue, suggesting
19 that the adsorption and desorption mechanism for the FD&C Blue may be singular as
20 compared to the Disperse Violets dual mechanism.

21 Flury and Fluhler (1995) imply that the adsorption and desorption of FD&C Blue
22 No. 1 are affected by the ion pairing with Ca^{2+} in soils, a finding supported by our data. A

1 change in pH effects little change in the adsorption of the FD&C Blue No. 1 on the
2 Accusand. However, the change in pH does effect the CEC of the Woodburn soil
3 system, and the adsorption of the FD&C Blue No. 1. This mechanistic explanation is
4 supported by the Accusand results, where at a pH 8 there is only 1.5% more adsorption of
5 the blue dye as compared to pH 4, and the Woodburn results where there is 50% more
6 adsorption at pH 8 than at pH 4. Butters and Bandaranayake (1993a) determined, by
7 using column studies, the retardation of FD&C Blue No. 1 to be slightly greater in fine
8 sand than in clay loam with organic matter. They tied this surprising result to the
9 movement of the blue dye with soluble organic matter in the clay loam. Adsorption due
10 to organic matter is excluded in our study due to the high solubility and the low K_{ow} of
11 FD&C Blue No. 1, leaving the CEC as the controlling factor of it's mobility through soil.

12 Our experiments using the Woodburn soil show hysteresis in the sorption process
13 with desorption isotherms having greater partitioning coefficients than the adsorption
14 isotherms for both dyes. The amount of energy it takes for the system to readjust to a
15 new equilibrium is evident in the curvilinear top of the regression curve for the desorption
16 isotherm (Fig. 3). Due to the similarity between the adsorption and desorption data
17 collected for the two dyes in the Accusand, the isotherms were not presumed to display
18 strong hysteretic effects (Table 3).

19

20 **Octanol/Water Partitioning**

21 The results from the octanol/water partitioning experiments provided a clear
22 contrast between the absorbency of the hydrophobic disperse violet dye and the

1 hydrophilic blue food coloring dye. The octanol/water partitioning coefficients (K_{ow}), of
2 Disperse Violet Dye No. 1 and FD&C Blue Dye No. 1 were 6.3×10^{-5} and 7.0×10^{-3}
3 respectively. The accuracy of the FD&C Blue results are low due to the difficulty in
4 measuring a molar absorbtivity coefficient (ϵ_{λ}), for the dye in octanol. Flury and Fluhler
5 (1994) estimated the K_{ow} for FD&C Blue to be $< 1.0 \times 10^{-4}$. Even with the variation
6 between the two results, both describe the incompatibility of FD&C Blue with organic
7 matter in a system. The large coefficient for the Disperse Violet dye clearly describes its
8 affinity for organic matter.

9

10 **Comparison to Predicted Values**

11 Our experimental results were compared to published empirical equations to assess the
12 usefulness of mathematical extrapolation to predict adsorption partitioning coefficients (K_d) for
13 these dyes (Table 4). The experimental K_d values for adsorption partitioning were
14 compared to calculated values of from an equation found in Rao and Davidson (1980)

$$15 \quad K_d = (f_{oc}) (K_{oc}). \quad [1]$$

16 This equation takes into consideration the percent of organic carbon content in the soil (f_{oc}
17 = organic carbon fraction) and the partitioning coefficient from water to organic carbon
18 (K_{oc}), calculated using the empirical relationship developed Krickhoff et al. (1979)

$$19 \quad K_{oc} = 0.411(K_{ow}) \quad [2]$$

20 Krickhoff's equation specifically defines hydrophobic pollutants in soils. Chiou (1990)
21 developed a relation using the solubility of the dye in water (S_w) in order to predict K_{ow}

$$22 \quad \text{Log } K_{ow} = -\text{Log } S_w + 0.92. \quad [3]$$

1 For aromatic liquids and solids the Chiou (1990) equation is

$$2 \quad \text{Log } K_{ow} = -0.862 \text{ Log } S_w + 0.71. \quad [4]$$

3 This equation 4 takes into consideration the aromatic configuration of chemicals as well as
4 their solubility in water. Equations [1] and [2] provide results that are inconsistent with
5 our experimental values for hydrophilic FD& C Blue No. 1; results differ by \geq five orders
6 of magnitude. However, for the hydrophobic Disperse Violet No. 1, these equations
7 provide results within one order of magnitude. Equation [4] provides the best fit for our
8 experimentally derived octanol/water partitioning coefficients; being within a factor of two
9 for the violet dye, and off by a factor of 8,000 for the blue dye.

10 The experimental results for FD&C Blue No. 1 and the Disperse Violet No. 1
11 differ from the calculated results by several orders of magnitude. These deviations
12 between the experimental K_{ow} and K_{oc} , and the calculated quantities often depend upon
13 structural differences and the exposure time of the dye to the organic matter (Mingelgrin and
14 Gerstl, 1983). The retardation factor (R), was calculated in order to assess the mobility of
15 a chemical through soil and assumes linear adsorption and fully reversible desorption.
16 The retardation factor describes the ratio of transport velocity of water to that of a
17 chemical through a soil. The equation which is used to calculate R requires K_d along with
18 the bulk density of the soil (ρ), and the soil/water content of the soil (θ) (Chiou, 1990),

$$19 \quad R = 1 + \rho(K_d)/\theta. \quad [6]$$

20 The bulk density and soil/water content for the Woodburn soil was determined to be 1.40 g
21 cm^{-3} and 0.2 g mL^{-1} respectively, and for the Accusand the bulk density and soil/water content

1 was estimated to be 1.3 g cm^{-3} and 0.6 g mL^{-1} respectively. The retardation factors for each
2 soil and dye are listed in Table 4; ranging from 5 to 1600.

4 CONCLUSION

5
6 Following a broad screening of seven potentially useful dye tracers, only FD&C Blue
7 Dye No. 1 and Disperse Violet Dye No. 1 were identified as likely candidates to use as
8 geohydrologic tracers to determine the mobility of organic chemicals through soil. Effects of
9 pH on tracer mobility were evident for both dyes as demonstrated during batch experiments
10 using Woodburn soil and Accusand. Cation exchange effects were evident for the
11 hydrophobic dye Disperse Violet No. 1 indicating a duo mechanism effecting the mobility of
12 the dye has as compared to a singular mechanism for the hydrophilic dye FD&C Blue No. 1.
13 Both dyes also demonstrated hysteretic effects between adsorption and desorption partition
14 coefficients.

15 These results indicate that Disperse Violet No. 1 is not an adequate tracer for field
16 studies due to its low solubility and high affinity for soil organic matter. Although the
17 experimental results were consistent, this dye would be virtually impossible to detect in a
18 field study because of small concentrations. The dye FD&C Blue No. 1 has the potential
19 to be an excellent field and laboratory tracer to mimic leaching chemicals. It's low
20 toxicity, high solubility and consistent experimental results prove FD&C Blue No. 1 to be
21 an ideal tracer.

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CAPTION PAGE

- Fig. 1: Chemical Structure for FD&C Blue No. 1
- Fig. 2: Chemical Structure for Disperse Violet No. 1
- Fig. 3: Adsorption and Desorption Isotherms for FD&C Blue No. 1 by the Woodburn soil sample at pH 8.0

1 **Table 1. Chemical and physical properties of Disperse dyes and FD&C Blue No. 1**

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3 Dyes and † CI #s	4 Molar Mass Sum formula	5 Solubility Water @ 25°C mol L ⁻¹	6 Absorption Max. nm	7 Absoptivity # (ε _λ) L mol ⁻¹ cm ⁻¹	
				8 Water	9 Octanol
10 Disperse Blue # 3 11 CI # 61505	12 296 13 C ₁₅ H ₁₆ N ₂ O ₃	14 1.2 X 10 ⁻⁷	15 587±03	16 ‡ NA	17 NA
18 Disperse Blue # 23 19 CI # 61545	20 326 21 C ₁₈ H ₁₈ N ₂ O ₄	22 3.1 X 10 ⁻⁰⁶	23 NA	24 NA	25 NA
26 Disperse Blue # 79 27 CI # 11345	28 625 29 C ₂₃ H ₂₅ BrN ₆ O ₁₀	30 1.0 X 10 ⁻⁹	31 NA	32 NA	33 NA
34 Disperse Violet # 1 35 CI # 61100	36 238 37 C ₁₂ H ₁₀ N ₂ O ₂	38 5.1 X 10 ⁻⁷	39 553±03	40 1.88 X 10 ⁺⁰⁸	41 7.67 X 10 ⁺⁰³
42 Disperse Violet # 8 43 CI # 62030	44 283 45 C ₁₂ H ₉ N ₃ O ₄	46 2.9 X 10 ⁻⁶	47 NA	48 NA	49 NA
50 Solvent Blue # 59 51 CI # 61552	52 294.36 53 C ₁₆ H ₁₈ N ₂ O ₂	54 not	55 642	56 NA	57 NA
58 FD&C Blue No. 1 59 CI # 42090	60 792.84 61 C ₃₇ H ₃₄ N ₂ Na ₂ O ₉ -S ₃	62 6.3 X 10 ⁻²	63 630±04	64 1.30 X 10 ⁺⁰⁵	65 § NA

27 † CI = Colour Index

28 ‡ NA = data not available

29 § Difficult to measure molar absorbtivity coefficient due to low solubility in octanol

1 **Table 2. Physical soil characteristics**

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Origin (soil texture)	pH	Organic	‡ CEC	Soil Texture		
		† Carbon		Clay	Silt	Sand
		%	cmol kg ⁻¹	%		
Woodburn Series Corvallis, OR (silty loam)	5.7	1.62	17.5	12	31	56
Accusand 30-40 Unimin Corp., MN (clean sand)	6.9	0.03	0.62	0	0	100

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15 † Expressed on dry soil weight basis

16 ‡ CEC = cation-exchange capacity

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1 **Table 3. Results of Partitioning Experiments for Disperse Violet No. 1 and FD & C Blue No. 1**

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4	Dye	Soil	pH	K_d	†R²	K_{ow}
5	FD&C Blue No. 1					
6	Adsorption	Accusand	4.0	1.12	0.96	
7		Accusand	8.0	1.77	0.99	
8		Woodburn	4.0	60.0	0.82	
9		Woodburn	8.0	30.0	0.93	
10	Desorption	Accusand	4.0	0.24	0.21	
11		Woodburn	8.0	61.0	0.72	
12		Woodburn	4.0	96.0	0.78	
13	Octanol/Water				0.78	7.0X10 ⁻³
14	Disperse Violet No. 1					
15	Adsorption	Accusand	4.0	1.38	0.30	
16		Accusand	8.0	2.38	0.70	
17		Woodburn	4.0	340.0	0.87	
18		Woodburn	8.0	227.0	0.59	
19	Desorption	Accusand	4.0	3.78	-0.28	
20		Woodburn	8.0	659.0	0.50	
21		Woodburn	4.0	587.0	-0.67	
22	Octanol/Water				0.89	6.3X10 ⁺⁵

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25 † Regression statistic

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1 **Table 4. Estimated Transport Coefficients**

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3 Dye	Soil	† K_{oc}	‡ K_d	§ K_{ow}	¶ K_{ow}	# R
4 FD&C Blue No. 1		2.88×10^{-3}		1.88×10^4	7.94×10^3	
	5 Accusand		8.67×10^{-7}			4.83
	6 Woodburn		4.66×10^{-5}			$4.21 \times 10^{+2}$
8 Disperse Violet No. 1		$2.60 \times 10^{+5}$		25.75	2.15	
	9 Accusand		78.0			6.16
	10 Woodburn		$4.21 \times 10^{+3}$			$1.59 \times 10^{+3}$

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12 † $K_{oc} = 0.411(K_{ow})$; K_{ow} = experimentally derived; Krickhoff et al., 1979

13 ‡ $K_d = (f_{oc})(K_{oc})$; $f_{oc} = \%OC/100$; Rao and Davidson, 1980

14 § Log K_{ow} estimated/ Log K_{ow} measured; Log $K_{ow} = -\text{Log } S_w + 0.92$; Chiou, 1990

15 ¶ Log K_{ow} estimated/ Log K_{ow} measured; Log $K_{ow} = -0.862 \text{ Log } S_w + 0.71$; Chiou, 1990

16 # $R = 1 + \rho K_d / \theta$; K_d = expermentally derived at pH 8; Chiou, 1990

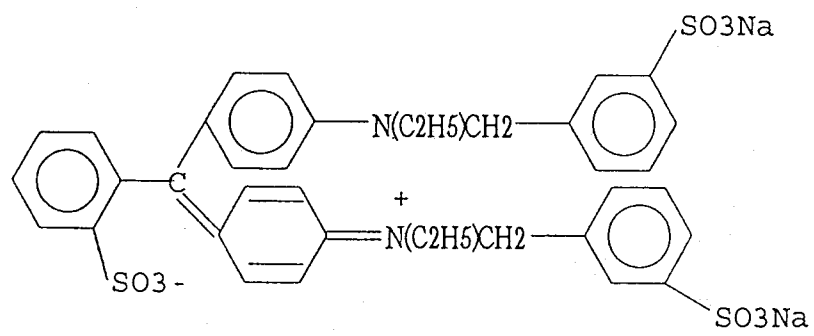


Figure 1

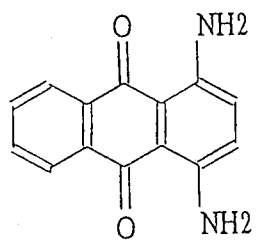


Figure 2

