

Screening Assessment for the Challenge

**9,10-anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)-
(Disperse Blue 77)**

**Chemical Abstracts Service Registry Number
20241-76-3**

**Environment Canada
Health Canada**

February 2009

Synopsis

Pursuant to section 74 of the *Canadian Environmental Protection Act, 1999* (CEPA 1999), the Ministers of the Environment and of Health have conducted a screening assessment on 9, 10-Anthracenedione, 1, 8-dihydroxy-4-nitro-5-(phenylamino)- (Disperse Blue 77), Chemical Abstracts Service Registry Number 20241-76-3. This substance was identified as a high priority for screening assessment and included in the Challenge because it had been found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms and is believed to be in commerce in Canada.

The substance Disperse Blue 77 was not considered to be a high priority for assessment of potential risks to human health, based upon application of the simple exposure and hazard tools developed by Health Canada for categorization of substances on the *Domestic Substances List*. Therefore, this assessment focuses on information relevant to the evaluation of ecological risks.

Disperse Blue 77 is an organic substance that is used in Canada and elsewhere as a blue colorant dye in textiles. The substance is not naturally produced in the environment. Disperse Blue 77 is not manufactured in Canada but between 100 and 1000 kg of Disperse Blue 77 were imported into Canada in 2006 for use mainly in the textile industry. The quantity of Disperse Blue 77 imported into Canada and the nature of its uses indicate that it could be released into the Canadian environment.

Based on certain assumptions and reported use patterns, most of the substance ends up in waste disposal sites (98.4%) while the remaining portion is estimated to be released to sewer water (1.6%) and air (0.1%). Disperse Blue 77 is not soluble in water, is not volatile and has a tendency to partition to particles and lipids (fat) of organisms because of its hydrophobic nature. For these reasons, Disperse Blue 77 is likely to be found mostly in sediments and, to a lesser extent, in soil. It is not expected to be significantly present in other media. It is also not expected to be subject to long-range atmospheric transport.

Based on its physical and chemical properties, Disperse Blue 77 does not degrade quickly in the environment and is therefore expected to be persistent in water, soil and sediments. Recent bioaccumulation data for Disperse Blue 77 and information for chemical analogues show that this substance does not have a high potential to accumulate in aquatic organisms. Disperse Blue 77 therefore meets the persistence criteria but does not meet the bioaccumulation criteria as set out in the *Persistence and Bioaccumulation Regulations*. Empirical acute aquatic toxicity values of analogues of Disperse Blue 77 suggest that the substance is not highly hazardous to aquatic organisms.

No environmental monitoring data relating to the presence of Disperse Blue 77 in the Canadian environment (air, water, soil, sediment) have been identified. For this screening assessment, a very conservative exposure scenario was designed in which it is assumed that all industrial operations (users of the dye) discharge Disperse Blue 77 into the

aquatic environment. The predicted environmental concentration in water was well below the predicted no-effect concentration calculated for sensitive aquatic organisms. Considering these findings, Disperse Blue 77 is unlikely to be causing ecological harm in Canada.

This substance will be included in the upcoming *Domestic Substances List* inventory update initiative. In addition and where relevant, research and monitoring will support verification of assumptions used during the screening assessment.

Based on the information available, it is concluded that Disperse Blue 77 does not meet any of the criteria set out in section 64 of CEPA 1999.

Introduction

The *Canadian Environmental Protection Act, 1999* (CEPA 1999) (Canada 1999) requires the Minister of the Environment and the Minister of Health to conduct screening assessments of substances that have met the categorization criteria set out in the Act to determine whether these substances present or may present a risk to the environment or human health. Based on the results of a screening assessment, the Ministers can propose to take no further action with respect to the substance, to add the substance to the Priority Substances List (PSL) for further assessment, or to recommend that the substance be added to the List of Toxic Substances in Schedule 1 of the Act and, where applicable, the implementation of virtual elimination.

Based on the information obtained through the categorization process, the Ministers identified a number of substances as high priorities for action. These include substances that

- met all of the ecological categorization criteria, including persistence (P), bioaccumulation potential (B) and inherent toxicity to aquatic organisms (iT), and were believed to be in commerce; and/or
- met the categorization criteria for greatest potential for exposure (GPE) or presented an intermediate potential for exposure (IPE), and had been identified as posing a high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity.

The Ministers therefore published a notice of intent in the *Canada Gazette*, Part I, on December 9, 2006 (Canada 2006), that challenged industry and other interested stakeholders to submit, within specified timelines, specific information that may be used to inform risk assessment, and to develop and benchmark best practices for the risk management and product stewardship of those substances identified as high priorities.

The substance 9, 10-Anthracenedione, 1, 8-dihydroxy-4-nitro-5-(phenylamino) - (Disperse Blue 77) was identified as a high priority for assessment of ecological risk as it was found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The Challenge for Disperse Blue 77 was published in the *Canada Gazette* on August 18, 2007 (Canada 2007). A substance profile was released at the same time. The substance profile presented the technical information available prior to December 2005 that formed the basis for categorization of this substance. As a result of the Challenge, submissions of information were not received.

Although Disperse Blue 77 was determined to be a high priority for assessment with respect to the environment, it did not meet the criteria for GPE or IPE and high hazard to human health based on classifications by other national or international agencies for carcinogenicity, genotoxicity, developmental toxicity or reproductive toxicity. Therefore, this assessment focuses principally on information relevant to the evaluation of ecological risks.

Under CEPA 1999 (Canada 1999), screening assessments focus on information critical to determining whether a substance meets the criteria for defining a chemical as toxic as set out in section 64 of the Act, where

- “64. [...] a substance is toxic if it is entering or may enter the environment in a quantity or concentration or under conditions that
- (a) have or may have an immediate or long-term harmful effect on the environment or its biological diversity;
 - (b) constitute or may constitute a danger to the environment on which life depends; or
 - (c) constitute or may constitute a danger in Canada to human life or health.”

Screening assessments examine scientific information and develop conclusions by incorporating a weight-of-evidence approach and precaution as required under CEPA 1999.

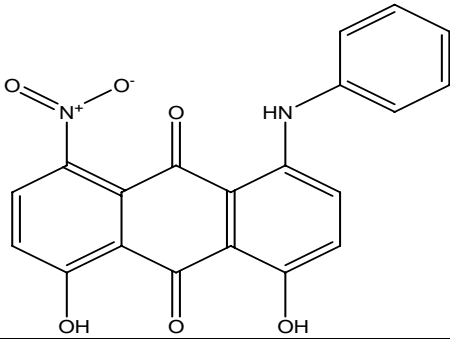
This screening assessment includes consideration of information on chemical properties, hazards, uses and exposure, including the additional information submitted under the Challenge. Data relevant to the screening assessment of this substance were identified in original literature, review and assessment documents, stakeholder research reports and from recent literature searches, up to July 2007. Key studies were critically evaluated; modelling results may have been used to reach conclusions. When available and relevant, information presented in hazard assessment from other jurisdictions was considered. The screening assessment does not represent an exhaustive or critical review of all available data. Rather, it presents the most critical studies and lines of evidence pertinent to the conclusion.

This screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. Additionally, the draft of this screening assessment was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening assessment remain the responsibility of Health Canada and Environment Canada. The critical information and considerations upon which the assessment is based are summarized below.

Substance Identity

For the purposes of this report, this substance will be referred to as Disperse Blue 77. “Disperse Blue 77” is defined by the Colour Index (CII 2002–) as a combination of multiple chemical abstracts service registry numbers (CAS RN), including CAS RN 20241-76-3. However, for the purposes of this document, the common name “Disperse Blue 77” refers exclusively to the CAS RN 20241-76-3.

Table 1. Substance identity of Disperse Blue 77

Chemical Abstracts Service Registry Number (CAS RN)	20241-76-3
DSL name¹	9,10-Anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)-
National Chemical Inventories (NCI) Inventory names²	9,10-anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)- (TSCA,, AICS, ASIA-PAC, NZIoC, PICCS) 1,8-dihydroxy-4-nitro-5-(phenylamino)anthraquinone (EINECS) Disperse Blue 120 (ENCS) Disperse Blue 77 (ENCS) C.I. disperse blue 077 (ECL)
Other names	1-Anilino-4,5-dihydroxy-8-nitroanthraquinone; 4-Anilino-5-nitro-1,8-dihydroxyanthraquinone; 4-Anilino-5-nitrochrysazin; 4-Nitro-5-anilinochrysazin; Anthraquinone, 1-anilino-4,5-dihydroxy-8-nitro- C.I. 60766; C.I. Disperse Blue 120; C.I. Disperse Blue 77; Eastman Polyester Blue BLF; Serilene Blue BLFS; Teratop Navy 2RLA
Chemical group (DSL stream)	Discrete organics
Chemical sub-group	Anthraquinone
Chemical formula	C ₂₀ H ₁₂ N ₂ O ₆
Chemical structure	
SMILES	O=C(c(c(c(O)cc1)C(=O)c2c(O)ccc3N(=O)(=O)c1Nc(ccc4)c4)c23
Molecular mass	376.323 g/mol

¹ DSL (Domestic Substances List).

² **Source:** National Chemical Inventories (NCI). 2007: AICS (Australian Inventory of Chemical Substances); ASIA-PAC (Asia-Pacific Substances Lists); ECL (Korean Existing Chemicals List); EINECS (European Inventory of Existing Chemical Substances); ENCS (Japanese Existing and New Chemical Substances); PICCS (Philippine Inventory of Chemicals and Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); TSCA (Toxic Substances Control Act Chemical Substance Inventory).

Physical and Chemical Properties

With the exception of physical state, no other experimental physical and chemical properties data are available for Disperse Blue 77. At the Environment Canada-sponsored Quantitative Structure-Activity Relationship (QSAR) Workshop in 1999 (Environment

Canada 2000), Environment Canada and other invited modelling experts identified many structural classes of pigment and dyes as being difficult to model using QSARs. The inherent properties of many of the structural classes of dyes and pigments (including acid and disperse dyes) are not amenable to model prediction because they are considered “out of the model domain of applicability” (e.g., structural and/or property parameter domains). Therefore, to determine the domain of applicability, Environment Canada reviews the applicability of QSAR models to dyes and pigments on a case-by-case basis. It has been considered inappropriate to use QSAR models to predict the physical and chemical properties of Disperse Blue 77 and consequently a “read-across” approach was used to determine the approximate physical and chemical properties in Table 2. These properties were subsequently used for further modelling in this assessment.

In order to find acceptable analogues, a review of data for several disperse anthraquinone dyes was performed (Anliker et al. 1981; Anliker and Moser 1987; Baughman and Perenich 1988; ETAD 1992, 1995; Brown 1992). These compounds have higher molecular weights, generally > 300 g/mol, have solid crystalline structures, decompose at greater than 220°C, and are dispersible in water (i.e. not truly soluble). In addition, they have limited solubility in n-octanol, a negligible vapour pressure and are stable under environmental conditions since they are designed to be so. These properties were subsequently used for further modelling in this assessment.

Table 2 below contains analogue as well as read-across experimental and calculated physical and chemical properties of Disperse Blue 77 that are relevant to its environmental fate.

Table 2. Physical and chemical properties for Disperse Blue 77

Property	Type ¹	Value	Temperature (°C)	Reference
Physical State	Experimental	Blue Powder		MSDS 1996
Melting point² (°C)	Read-across	225		Anliker and Moser 1987
		~ 130 to 330		Baughman and Perenich 1988
Boiling point³ (°C)	Not applicable			
Density (kg/m³)	Not available			
Vapour pressure (Pa)	Read-across	2.7×10^{-11} to 1.3×10^{-4} (2×10^{-13} to 10^{-6} mm Hg)	25	Baughman and Perenich 1988
Henry's Law constant (Pa·m³/mol)	Read-across ⁴	10^{-9} to 10^{-1} (10^{-14} to 10^{-6} atm m ³ /mol)		Baughman and Perenich 1988

Property	Type ¹	Value	Temperature (°C)	Reference
Log K_{ow} (Octanol-water partition coefficient) (dimensionless)	Analogue Disperse Violet 26	5.1 ⁵		ETAD 1992
	Analogue Disperse Blue 60	4.1		
	Analogue Disperse Blue 73	3.4		
	Read-across	> 4		Anliker et al. 1981 Anliker and Moser 1987
Log K_{oc} (Organic carbon partition coefficient) (dimensionless)	Read-across, calculated ⁶	3.4 to 4.2		Baughman and Perenich 1988
Water solubility (mg/L)	Read-across	< 0.01	20	Anliker and Moser 1987
		substantially water insoluble		ETAD 1995
	Analogue Disperse Violet 26	Insoluble		ETAD 1992
	Analogue Disperse Blue 60	0.0 ² (2 × 10 ⁻⁵ g/L) ⁷		
	Analogue Disperse Blue 73	0.2 (2 × 10 ⁻⁴ g/L)		
n-octanol solubility (mg/L)	Read-across	120	20	Anliker and Moser 1987
pK_a (Acid dissociation constant)	Modelled	3.93 for base form		ACD/pK _a DB 2005

Property	Type ¹	Value	Temperature (°C)	Reference
(dimensionless)				

¹ The extrapolated values used for Disperse Blue 77 are based on evidence on disperse dyes submitted to Environment Canada under the *New Substances Notification Regulations* (ETAD 1995) and available evidence from other disperse dye analogues found in literature.

² The phrase “melting point” is used but this may be better referred to as a “decomposition point” because disperse dyes are known to char at high temperatures (greater than 200°C) rather than melt.

³ “Boiling point” is generally not applicable for disperse dyes. For powder dyes, charring or decomposition occurs at high temperatures instead of boiling. For liquids and pastes, boiling will only occur for the solvent component, while the unevaporated solid will decompose or char (ETAD 1995).

⁴ Solubilities of several disperse dyes at 25 and 80°C were used by Baughman and Perenich (1988) to calculate Henry’s Law constants for these dyes. These values are presented here as a range to illustrate the expected Henry’s Law constant for Disperse Blue 77.

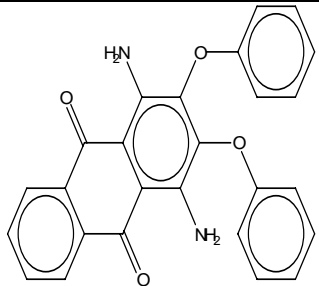
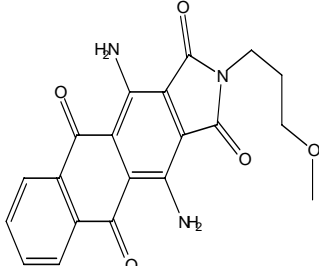
⁵ Log K_{ow} was obtained using the HPLC method.

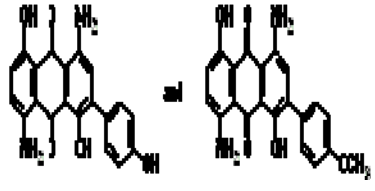
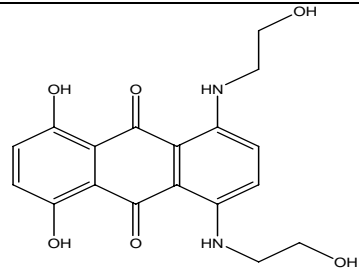
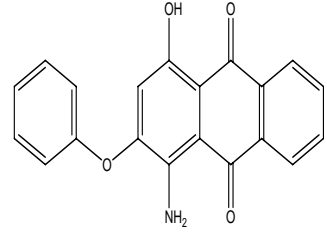
⁶ Log K_{oc} values are based on calculations by Baughman and Perenich (1988) using a range of measured solubilities for commercial dyes and an assumed melting point of 200°C.

⁷ Tested as active ingredient (FAT-36’ 152/C) and not as dispersion.

Structural disperse anthraquinone analogues to Disperse Blue 77 are presented in Table 3 below. Certain physical and chemical properties (Table 2), empirical bioaccumulation data (Table 6) and empirical toxicity data (Table 7) of these analogues were used in support of the weight of evidence and proposed decisions in this screening assessment report. Specifically, physical and chemical properties were obtained for the following structural analogues: (i) Disperse Violet 26, (ii) Disperse Blue 60 and (iv) Disperse Blue 73. Empirical toxicity data were obtained for: (i) Disperse Violet 26, (iii) Disperse Blue 73, (iv) Disperse Blue 7 and (v) Disperse Red 60.

Table 3a. Structural analogues for Disperse Blue 77

	CAS RN* or Colour index number**	Common name	DSL name ¹	Structure of analogue
i.	6408-72-6*	Disperse Violet 26	9,10-Anthracenedione, 1,4-diamino-2,3-diphenoxy-	
ii.	61104**	Disperse Blue 60	1H-Naphth[2,3-f]isoindole-1,3,5,10(2H)-tetrone, 4,11-diamino-2-(3-methoxypropyl)-	

	CAS RN* or Colour index number**	Common name	DSL name ¹	Structure of analogue
iii.	63265**	Disperse Blue 73	Not applicable as this is a mixture of methoxy and hydroxy forms	
iv.	3179-90-6*	Disperse Blue 7	9,10-Anthracenedione, 1,4-dihydroxy-5,8-bis[(2-hydroxyethyl)amino]-	
v.	17418-58-5*	Disperse Red 60	9,10-Anthracenedione, 1-amino-4-hydroxy-2-phenoxy-	

¹ Source: National Chemical Inventories (NCI) 2007: Canadian Domestic Substances List (DSL).

It should be noted that there are several uncertainties associated with the use of physical, chemical and toxicological data and bioaccumulation data available for the substances presented in Table 3a. All these substances share the same chemical class, disperse anthraquinone dyes (with their characteristic three-ring structure with two sets of double-bond oxygen atoms off the middle ring), have similar molecular weights and are used for similar industrial purposes. However, there are differences between these substances associated with their unique functional groups (see Table 3b below). As a result, these analogues have different empirical water solubilities that range from 0.0² to 0.2 mg/L and empirical log K_{ow} values that vary over almost 3 orders of magnitude from 3.4 and 5.1 (see Table 2 above). Due to this variability, which cannot be easily interpreted, caution should be exercised in attributing too much weight to these values as it would be preferable to utilize empirical water solubility and a log K_{ow} specific to the substance Disperse Blue 77.

Table 3b. Comparisons of structural analogues with Disperse Blue 77

	CAS RN* or Colour Index number**	Common name	Comparison with Disperse Blue 77
i.	6408-72-6*	Disperse Violet 26	Contains two extra phenyloxy and two primary amines on the anthraquinone structure. Lacks a nitro, a phenylamine and two alcohol groups on the anthraquinone structure.
ii.	61104**	Disperse Blue 60	Contains one extra cyclic amide and two primary amines on the anthraquinone structure. Lacks a nitro, a phenylamine and two alcohol groups on the anthraquinone structure.
iii.	63265**	Disperse Blue 73	Contains one extra anisole or phenol, one hydroxyl and two primary amines on the anthraquinone structure. Lacks a nitro, a phenylamine and one alcohol groups on the anthraquinone structure.
iv.	3179-90-6*	Disperse Blue 7	Contains two extra 2-aminoethanol and one hydroxyl on the anthraquinone structure. Lacks a nitro, a phenylamine and two alcohol groups on the anthraquinone structure.
v.	17418-58-5*	Disperse Red 60	Contains one extra phenyloxy and one primary amine on the anthraquinone structure. Lacks a nitro, a phenylamine and two alcohol groups on the anthraquinone structure.

Sources

Disperse Blue 77 is not naturally produced in the environment.

Recent information was collected through an industry survey conducted for the years 2005 and 2006 under *Canada Gazette* notices issued pursuant to section 71 of CEPA 1999 (Canada 2006, 2007). These notices requested data on the Canadian manufacture, import and use of the substance.

In 2006, two companies reported importing this substance, and collectively they imported between 100 and 1000 kg of the substance. No companies reported manufacturing Disperse Blue 77 in Canada above the prescribed reporting threshold of 100 kg/year for that year. No companies reported using a total quantity greater than 1000 kg of the substance, whether alone, in a mixture, in a product or in a manufactured item, at any concentration in 2006. In the Declaration of Stakeholder Interest form associated with the section 71 notice for 2006, four companies reported a stakeholder interest in this substance despite not meeting mandatory reporting requirements (Environment Environment Canada. 2008a). 2007a).

Two companies reported importing a total of between 100 and 1000 kg of the substance in 2005. These companies were different from those that reported in year 2006. No companies reported manufacturing Disperse Blue 77 in Canada above the prescribed reporting threshold of 100 kg/year for that year. No companies reported using a total quantity greater than 1000 kg of the substance, whether alone, in a mixture, in a product or in a manufactured item, at any concentration in 2005. No companies identified

themselves as having a stakeholder interest in the substance in 2005 (Environment Canada 2006).

In the United States, between 4500 and 225 000 kg of Disperse Blue 77 were manufactured and/or imported in each of the following years: 1986, 1990, 1994, 1998 and 2002 (US EPA 2007). Disperse Blue 77 is an existing chemical in Europe, but is not on the low or high production volume chemicals lists (ESIS 2007). The database for Substances in Preparations in Nordic Countries indicates that, in 2005, approximately 8.5 tonnes were used in Denmark, 0.1 tonnes were used in Finland and 2 tonnes were used in Sweden (SPIN 2007).

Uses

Recent use information was collected through an industry survey conducted for the years 2005 and 2006 (Environment Canada 2006 and 2007a); however, this cannot be disclosed as it has been designated confidential. Despite its confidentiality, this information was taken into consideration in the assessment.

The following use codes were specified for the substance during the DSL nomination (1984–1986): “Colorant- pigment/stain/dye/ink”; “Textile, primary manufacture”; and “Textile, product.”

No other uses of Disperse Blue 77 in Canada were identified through searches of the available scientific and technical literature. Disperse Blue 77 was used in the textile industry in Denmark, Sweden and Finland in the years 2000–2005 (SPIN 2007).

Releases to the Environment

Mass Flow Tool

To estimate potential releases of the substance to the environment at different stages of its life cycle, a Mass Flow Tool was developed (Environment Canada 2008b). Empirical data concerning releases of specific substances to the environment are seldom available. Therefore, for each identified type of use of the substance, the proportion and quantity of release to the different environmental media are estimated, as is the proportion of the substance chemically transformed or sent for waste disposal. Unless specific information on the rate or potential for release of the substance from landfills and incinerators is available, the Mass Flow Tool does not quantitatively account for releases to the environment from disposal.

Assumptions and input parameters used in making the release estimates are based on information obtained from a variety of sources including responses to regulatory surveys, Statistics Canada, manufacturers’ websites and technical databases and documents. Of particular relevance are emission factors, which are generally expressed as the fraction of a substance released to the environment, particularly during its manufacture, processing,

and use associated with industrial processes. Sources of such information include emission scenario documents, often developed under the auspices of the Organisation for Economic Co-operation and Development (OECD) and default assumptions used by different international chemical regulatory agencies. It is noted that the level of uncertainty in the mass of substance and quantity released to the environment generally increases towards the end of the life cycle.

Table 4. Estimated releases and losses of Disperse Blue 77 to environmental media, chemical transformation and distribution to management processes, based on the Mass Flow Tool

Fate	Proportion of the mass (%) ¹	Major life cycle stage involved ²
Released to receiving media:		
Soil	0.0	Industrial use, consumer use
Air	0.1	-
Sewer ³	1.6	Formulation, industrial use, consumer use
Chemically transformed	0	-
Transferred to waste disposal sites (e.g., landfill, incineration)	98.4	Formulation, industrial use, consumer use, waste disposal

¹ For Disperse Blue 77, information from the following OECD emission scenario documents was used to estimate releases to the environment and the distribution of the substance as summarized in this table: Coating Industry (OECD 2006) and Adhesive Formulation (OECD 2007). Values presented for release to environmental media do not account for possible mitigation measures that may be in place at some locations (e.g., partial removal by sewage treatment plants). Specific assumptions used in the derivation of these estimates are summarized in Environment Canada (2007b).

² Applicable stage(s): formulation-industrial use-consumer use-service life of article/product-waste disposal.

³ Wastewater before any form of treatment.

Results indicate that Disperse Blue 77 can be expected to be found largely in waste management sites (98.4%), due to the eventual disposal of manufactured items containing it. Mass Flow Tool calculations do not quantitatively account for releases of the substance to the environment from waste disposal sites (such as landfills, incinerators) unless specific information on the rate or potential for release is available. No such information has been identified for Disperse Blue 77. A small fraction of solid waste is incinerated, which is expected to result in transformation of the substance. Based largely on information contained in OECD emission scenario documents for processing and uses associated with this substance, it is estimated that 1.6%, 0% and 0.1% of Disperse Blue 77 may be released to sewer, soil and air, respectively.

Based on the above, wastewater is the environmental medium receiving the greatest amount of Disperse Blue 77 emitted during product processing and to a lesser extent consumer use of products containing this substance. It is anticipated that the majority of the substance bound in products will be sent to landfills for disposal.

Although no information is available on the total quantity of importation of consumer products containing Disperse Blue 77, it is anticipated that the proportions of releases to the various environmental media would not be significantly different from those estimated here. However, the quantities sent for waste management would be higher if importation of these products were taken into consideration.

Environmental Fate

According to the results of the Mass Flow Tool (Table 4), the substance Disperse Blue 77 is expected to be released to wastewater effluents during industrial processing and use.

Disperse Blue 77 is a dense solid particle. Like other disperse dyes it is expected to have a limited water solubility (see Table 2), although there is some uncertainty about this because the pKa for this substance of 3.93 (see Table 2) suggests it will ionize in solution. Therefore, when released into water, this substance is expected to eventually sink to bed sediments where it is expected to behave as a particle rather than a soluble organic chemical. It has been concluded by Yen et al. (1989) that disperse dyes tend to accumulate extensively in sediments and biota unless they are degraded at rates comparable to uptake.

The moderate to high log K_{ow} (analogues 3.4, 4.1, 5.1 and read across > 4) and high log K_{oc} (3.4 to 4.2) values (see Table 2) indicate that dissolved forms of this substance may have affinity for solids containing organic carbon. However, the log K_{oc} is a calculated value (see footnote 3 below Table 2) and most of this substance is expected to be present in water in the solid crystalline state, the degree to which Disperse Blue 77 is adsorbed to solids in the environment could be considerably less than suggested by available K_{ow} and K_{oc} information for analogues.

The rate of volatilization is proportional to the Henry's Law constant (Baughman and Perenich 1988). The low to negligible read-across Henry's Law constant value (10^{-9} to $0.1 \text{ Pa}\cdot\text{m}^3/\text{mol}$, Table 2) and vapour pressure indicates that Disperse Blue 77 is essentially non-volatile. Therefore, volatilization is not likely to be an important transport pathway for the loss of this substance from moist and dry soil surfaces as well as aquatic compartments.

Finally, air is not considered to be an important medium for Disperse Blue 77 due to the low volatility of this substance, as indicated by the low to negligible read-across vapour pressure (2.7×10^{-11} to $1.3 \times 10^{-5} \text{ Pa}$, Table 2) and Henry's Law constant. These data are consistent with the physical state (solid crystalline structure) of Disperse Blue 77, which does not make it a likely candidate for volatilization or significant transport in air..

Persistence and Bioaccumulation Potential

Environmental Persistence

No environmental monitoring data relating to the presence of Disperse Blue 77 in the Canadian environment (air, water, soil, sediment) have been identified. Furthermore, no experimental biological degradation data for Disperse Blue 77 have been identified.

According to the Ecological and Toxicological Association of Dyes and Organic Pigments Manufacturers, with some exceptions, dyes are considered essentially non-biodegradable under aerobic conditions (ETAD 1995). Repeated evaluation of ready and inherent biodegradability using accepted screening tests (see the *OECD Guidelines for the Testing of Chemicals* website) have confirmed this assumption (Pagga and Brown 1986; ETAD 1992). Based on the chemical structure of Disperse Blue 77, there is no reason to suspect that biodegradation will be other than that described for dyes (ETAD 1995). As described below, modelled data in Table 5 support this assumption of non-degradability.

Given the expected environmental fate of Disperse Blue 77 after release into wastewater and the ecological importance of this compartment, persistence was primarily examined using predictive QSAR models for biodegradation in water. The following analysis applies primarily to the portion of this substance that is present in the environment in dissolved form, recognizing that a significant proportion would also likely exist in the solid crystalline state. Disperse Blue 77 does not contain functional groups expected to undergo hydrolysis (dyes are designed to be stable in aqueous conditions).

Table 5. Modelled data for biodegradation of Disperse Blue 77

Model	Model basis	Medium	Value	Interpretation	Extrapolated half-life (days)	Extrapolation reference and/or source
BIOWIN1* v4.1 (2000)	Linear probability	water (aerobic)	0.40	Does not biodegrade fast	n/a	
BIOWIN2* v4.1 (2000)	Non-linear probability	water (aerobic)	0.02	Does not biodegrade fast	n/a	
BIOWIN3* v4.1 (2000)	Expert Survey (ultimate biodegradation)	water (aerobic)	2.15	Months	60	US EPA 2002
BIOWIN4* v4.1 (2000)	Expert Survey (primary biodegradation)	water (aerobic)	3.13	Weeks	15	US EPA 2002
BIOWIN5* v4.1 (2000)	MITI linear probability	water (aerobic)	-0.316	Does not biodegrade fast	n/a	
BIOWIN6* v4.1 (2000)	MITI non-linear	water (aerobic)	0.0003	Does not biodegrade fast	n/a	

Model	Model basis	Medium	Value	Interpretation	Extrapolated half-life (days)	Extrapolation reference and/or source
	probability					
BIOWIN7* v4.1 (2000)	Linear probability	anaerobic	-0.91	Does not biodegrade fast		
BIOWIN Overall conclusion ¹	BIOWIN 3 + BIOWIN 5	water (aerobic)	no	Not ready biodegradable	n/a	
CATABOL v. 5.100 (c2004–2008)	% BOD (OECD 301C)	water (aerobic)	0	Persistent (< 20%)	> 182	First-order-rate kinetics

*BIOWIN 1–7 are outputs obtained from the predictive model BIOWIN (2000). BIOWIN estimates aerobic and anaerobic biodegradability of organic chemicals using seven different models.

¹Based on outcome of BIOWIN 3 and BIOWIN 5.

The results from Table 5 show that the majority of the probability models (BIOWIN 1, 2, 5, 6 and 7) suggest this substance does not biodegrade fast. In fact, all probability results (except the one for BIOWIN1) are less than 0.3, the cut-off suggested by Aronson et al. (2006) below which substances are expected to have a half-life > 60 days (based on the MITI probability models) and the BIOWIN1 result is less than 0.5, the cut-off suggested by the model developers below which biodegradation is not considered to be fast. The half-life from the primary survey model (BIOWIN 4) result of “weeks” is suggested to mean approximately 15 days (US EPA 2002, Aronson et al. 2006), although the identity of potential degradation products is not known. The ultimate survey model (BIOWIN 3) result of “months” is suggested to mean approximately 60 days by the US EPA (2002) and 120 days by (Aronson et al. 2006). The substance is also not expected to degrade rapidly under anaerobic conditions. The overall conclusion from BIOWIN (2000) is that this substance is not ready biodegradable.

Another ultimate degradation model CATABOL, predicted a 0% biodegradation based on the OECD 301 28-day ready biodegradation test (% BOD), which has been suggested as meaning likely persistent (Aronson and Howard 1999) and having a half-life in water of > 182 days (assuming first-order-rate kinetics).

When the results of the BIOWIN models and CATABOL are considered, the weight of evidence suggests that the ultimate degradation half-life in water is > 182 days, which is consistent with what would be expected for a chemical used as a disperse dye. Although it is possible that this substance will undergo faster primary degradation (based on results of BIOWIN 4), there are significant uncertainties (e.g., dyes are manufactured to be relatively insoluble and durable), and there is no information on the identity of possible degradation products.

Using a 1:1:4 for a water:soil:sediment half-life extrapolation (Boethling et al. 1995), the ultimate degradation half-life in soil is also > 182 days and the half-life in sediments is > 365 days.

Based on the results of predictive modelling, Disperse Blue 77 meets the persistence criteria for water and soil (half-life in soil and water ≥ 182 days) as well as sediments (half-life in sediments ≥ 365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

A recent empirical bioconcentration test of Disperse Blue 77 in fish was submitted to Environment Canada (Hu and Shen 2008). This test was performed according to the *OECD Guidelines for the Testing of Chemicals*, Test No. 305B-1996. The bioconcentration of Disperse Blue 77 in Zebra fish (*Brachydanio rerio*) was determined in a 28-day semi-static test with a test medium renewal every two days. An exposure test at a nominal concentration of 20 mg/L (mean measured concentration <0.023 mg/L) was performed in accordance with the result of the fish acute toxicity test to check the bioconcentration potential of the test substance. Samples from both test solutions and test organisms were taken daily from the 26th day to the last day during the 28-day exposure test period. Samples were prepared by extracting the lipid component from the test fish. The measured concentration of test substance, fish lipid content and bioconcentration factor (BCF) calculations are reported in Table 6.

Table 6. Measured concentration of Disperse Blue 77, fish lipid content and BCF calculation

		Sampling time		
		26 th day	27 th day	28 th day
Treatments (20 mg/L)	Measured concentration of the test substance in extracted solutions (mg/L)	< 0.02	< 0.02	< 0.02
	Content of the test substance in the fish lipids (mg)	< 0.002	< 0.002	< 0.002
	Fish total weight (g)	3.07	3.47	3.11
	Concentration of the test substance in the fish C_f (mg/kg)	< 0.65	< 0.58	< 0.64
	Measured concentration of the test substance in the water C_w (mg/L)	< 0.023	< 0.023	< 0.023
	Fish lipid content (%)	1.37	1.95	1.47
	BCF	< 100	< 100	< 100
	Average BCF	< 100		

The Hu and Shen (2008) study has been reviewed and considered acceptable (see Appendix 1). Lack of detection in fish extracts (< 0.02 mg/L) suggests a limited solubility in lipids and/or limited potential to partition into fish tissue from aqueous systems—more likely both. However, there is some uncertainty associated with limit-bounded values in any study because the true value is not known.

Given the structure of the substance and the likely behaviour of this class of disperse dye in aqueous systems, a low BCF result would be expected. Most disperse dyes, as their

name would suggest, exist as fine dispersible particles with limited truly soluble fractions. Solubility, however, can be increased by adding polar functional groups to the molecule. Disperse Blue 77 contains some of these solubilizing groups (nitro and phenolic groups) and has a pKa suggesting potential for ionization in solution, thus some degree of water solubility would be expected. But, given a melting point of $\sim 225^{\circ}\text{C}$, the predicted water solubility (WSKOWIN) without accounting for ionization and corrected for melting point is ~ 0.01 mg/L, which is just slightly below the aqueous detection limit in the study and is in agreement with the analogue experimental value of 0.05 mg/L reported by Baughman and Perenich (1988). Using a water solubility of 0.01 mg/L and using the fish concentration of < 0.65 mg/kg, the BCF may be calculated to be < 100 .

Anliker et al. (1981) also report results from experimental fish bioaccumulation tests for disperse anthraquinone dyes, performed according to test methods specified by the Japanese Ministry of International Trade and Industry (MITI). The value reported represents pooled results from several unspecified disperse anthraquinone dyes obtained by the ETAD member companies seeking to register new dyestuffs in Japan. The reported log bioaccumulation factor (BCF) is < 0.7 ($\text{BCF} < 5$), and it is expressed on the basis of wet body weight of the fishes (Anliker et al. 1981; Anliker and Moser 1987). The reason for the apparent discrepancy between the moderate to high $\log K_{ow}$ and low log BCF values reported by Anliker et al. (1981) is unknown. The authors suggest that the high molecular weight of disperse dyestuffs (at 450–550 g/mol) may make transport across the fish membranes difficult. It is also likely that the lack of bioavailability and limited capacity to partition under BCF test conditions limits accumulation in fish lipids.

Disperse dyes, including the class of anthraquinones, have been shown to have partition coefficients and solubilities of a magnitude that, when taken alone, suggest a significant potential for bioaccumulation (Baughman and Perenich 1988). The experimental read-across $\log K_{ow}$ value for disperse anthraquinone-type dyes is > 4 , 5.1, 4.1 (Anliker et al 1981; Anliker and Moser 1987; ETAD 1992, see Table 2). These values indicate that Disperse Violet 57 may have the potential to bioaccumulate in organisms according to the $\log K_{ow}$ value alone. However, it is likely a limit value (reflecting a limit of detection in water and thus an unknown upper limit of $\log K_{ow}$). Additionally, high $\log K_{ow}$ of 5.1 may be questioned as it was experimentally derived using a procedure called high-performance liquid chromatography (HPLC). HPLC is sometimes criticized as a method to derive $\log K_{ow}$ data, as it depends upon the relationship between the studied substance and a similar chemical standard. Unfortunately, few if any HPLC standards exist for pigments and dyes. Also, this method is often used when the substance in question is so insoluble that a traditional $\log K_{ow}$ test is not possible. Without more detailed analytical information, it is difficult to ensure that this high $\log K_{ow}$ value is a credible value. The other two $\log K_{ow}$ values (3.4 and 4.1) seem more reasonable, given the other physical and chemical characteristics of disperse dyes, but are also not completely reliable given lack of information regarding the calculation method. In view of this, and the fact that this substance may ionize in solution, there is uncertainty associated with these data and it is difficult to determine bioaccumulation potential solely from these $\log K_{ow}$ values or when using it in bioaccumulation models.

For both their log K_{ow} and log BCF values, Anliker et al. (1981) do not report the experimental details, the identities of the dyes nor their corresponding Chemical Abstracts Service registry numbers (CAS RNs). This adversely affects the utility of these data. However, as little bioaccumulation data have been identified for disperse anthraquinone dyes in general, these data are nevertheless still considered for determining the bioaccumulation potential of Disperse Blue 77. The uncertainty inherent in the Anliker and Anliker and Moser data results in a lower weight being given to these results.

It has been concluded by Anliker and Moser (1987) that, for disperse dyes with substantially higher octanol solubilities, low water solubilities < 2 mg/L and relatively high log $K_{ow} > 3$, bioaccumulation may reach such high levels that they may warrant the execution of a fish accumulation test. The BCF study from Hu and Shen (2008) has addressed this need.

It has been stated by ETAD (1995) that the molecular characteristics indicating the absence of bioaccumulation are a molecular weight of > 450 g/mol and a cross-sectional diameter of > 1.05 nm. Recent investigation by Dimitrov et al. (2002), Dimitrov et al. (2005) and the BBM (2008) suggests that the probability of a molecule crossing cell membranes as a result of passive diffusion declines significantly with increasing maximum cross-sectional diameter (D_{max}). The probability of passive diffusion lowers appreciably when cross-sectional diameter is $> \sim 1.5$ nm and more significantly so for molecules having a cross-sectional diameter of > 1.7 nm. Sakuratani et al. (2008) have also investigated the effect of cross-sectional diameter on passive diffusion from a test set of about 1200 new and existing chemicals also observing that substances not having a very highly bioconcentration potential often have a $D_{max} (> 2.0$ nm) and an effective diameter ($D_{eff} > 1.1$ nm).

Disperse Blue 77 has a molecular weight of 376.323 g/mol and its molecular structure (see Table 1) is relatively uncomplicated; both these characteristics indicate some bioaccumulation capability for this substance if molecular weight is used as the indicator. However, an Environment Canada (2003) report points out that there is no clear basis for establishing strict molecular size cut-offs (mass or diameter-based) for assessing bioaccumulation potential. Arnot (2007) nevertheless acknowledges that it is likely that certain large molecules are poorly adsorbed. In this context it may be noted the maximum diameter of Disperse Blue 77 and its conformers ranges from 1.28 to 1.55 nm (BBM 2008), which is within the range of diameters reported to be associated with slow bioaccumulation by Dimitrov (2005), suggesting that a potential for a reduced uptake rate and in vivo bioavailability exists with this dye.

Bioaccumulation modelling was not performed for Disperse Blue 77. Many higher molecular weight pigments and non-soluble dye classes, including anthraquinone disperse dyes, are considered as difficult to model and thus the results are generally deemed unreliable. Important predicted and/or empirical properties of disperse dyes for predicting bioaccumulation (i.e., log K_{ow}) can be associated with a high degree of error, which would be transferred to model predictions of BCF and BAF. In addition,

anthraquinone disperse dyes fall outside of bioaccumulation model domains of applicability.

Considering the information discussed above, there is uncertainty regarding the bioaccumulation potential of Disperse Blue 77. Evidence is presented that both supports and argues against the substance having a high bioaccumulation potential. However, greatest reliability and thus weight has been assigned to the low empirical BCF value for Disperse Blue 77 itself, estimated from the data of Hu and Shen (2008). Although given lower weight due to lack of sufficient study details and the fact that the chemicals tested were structural analogues, the low BCF result from Anliker et al. (1981) and Anliker and Moser (1987) supports this conclusion. The potential for reduced uptake according to maximum cross-sectional diameter is also important and agrees with the BCF results. The only evidence for a higher bioaccumulation potential comes from one unbounded log K_{ow} value for a three relatively high log K_{ow} values for two structural analogue substances (4.1 and 5.1) and one unbounded log K_{ow} value from Anliker (1981), which was also given a low overall weight relative to the evidence from the empirical BCF study with Disperse Blue 77. Therefore, considering the overall weight of evidence, Disperse Blue 77 does not to meet the bioaccumulation criterion (BCF, BAF \geq 5000) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

A - In the Aquatic Compartment

Few empirical ecotoxicity data were identified for Disperse Blue 77. According to a Material Safety Data Sheet (1996), a 96-hr LC_{50} of 460 mg/L for Zebra fish and a 3-hr IC_{50} of 400 mg/L in a bacteria respiration inhibition test have been obtained experimentally (Table 7a). However, the original studies have not been provided to allow verification of their reliability.

Table 7a. Empirical data for aquatic toxicity of Disperse Blue 77

Test organism	Type of test	Duration (hours)	Endpoint	Reliability of the study	Value (mg/L)	Reference
Zebra fish	Acute	96	LC_{50} ¹	Not available	460	MSDS 1996
Bacteria (activated sludge)	Activated sludge respiration inhibition test	3	IC_{50} ²	Not available	400	MSDS 1996

¹ LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.

² IC_{50} – The concentration of a substance that is estimated to cause inhibition of 50% of the test organisms.

Two suitable analogues of Disperse Blue 77 (Disperse Blue 7 and Disperse Red 60) were also located in the ECOTOX (ECOTOX 2008) ECOTOX database. (2008) (Table 7b)

shows that the toxicity of these analogues is in the moderate to low range (52 to > 180 mg/L). The toxicity of Disperse Blue 77 is expected to be similar to that of the analogues due to comparable molecular size/weight, solubility. Therefore, these values would also suggest that Disperse Blue 77 is not hazardous to aquatic organisms at relatively low concentrations (i.e., acute $LC_{50} > 1$ mg/L).

In another study, a summary of which was submitted to Environment Canada on behalf of ETAD (Brown 1992), 11 disperse dyes were tested on the following organisms: Zebra fish, *Daphnia magna*, algae and bacteria. From the 11 disperse dyes tested by ETAD (1992), three are anthraquinone analogues of Disperse Blue 77 (ETAD 1992). These are Disperse Violet 26, Disperse Blue 73 and Disperse Blue 60. However, the aquatic toxicity data available for Disperse Blue 60 were considered unacceptable for presentation in the screening assessment due to ambiguity in the reported values. Data obtained for Disperse Violet 26 and Disperse Blue 73 are presented in Table 7b.

The experimental details for the dyes tested were not provided, greatly limiting evaluation of these studies. However, these data were considered usable and are included in this screening assessment as contributing to the weight of evidence. The three Disperse Blue 77 analogues tested show low toxicity to *D. magna* (48-hr $EC_{50} \geq 200$ mg/L) and low toxicity to Zebra fish (96-hr $LC_{50} \geq 122$ mg/L). These values would also therefore suggest that Disperse Blue 77 is not hazardous to aquatic organisms at relatively low concentrations (i.e., acute $LC_{50} > 1$ mg/L).

Table 7b. Empirical data for aquatic toxicity of Disperse Blue 77 analogues

Common name	Test organism	Endpoint	Value (mg/L)	Reference
Disperse Violet 26	Zebra fish	96-hr LC_{50} ¹	> 500 (no effect)	ETAD 1992
	<i>Daphnia magna</i>	48-hr EC_{50} ²	> 200 (no effect)	
Disperse Blue 73	Zebra fish	96-hr LC_{50}	> 500 (no effect)	
	<i>Daphnia magna</i>	48-hr EC_{50}	200	
Disperse Blue 7	Fathead minnow (<i>Pimephales promelas</i>)	24-hr LC_{50}	> 180 (no effect)	Little et al. 1974
		48-hr LC_{50}	142	
		96-hr LC_{50}	52	
		96-hr LC_{50}	52	Little and Lamb 1973
Disperse Red 60	Fathead minnow (<i>Pimephales promelas</i>)	LC_{50} (24-hr, 48-hr, 96-hr LC_{50})	> 180 (no effect)	Little et al. 1974
		96-hr LC_{50}	> 180 (no effect)	Little and Lamb 1973

¹ LC_{50} – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.

² EC_{50} – The concentration of a substance that is estimated to cause some toxic sublethal effect on 50% of the test organisms.

In general, due to their poor solubility (< 1 mg/L) and low bioaccumulation potential, disperse dyes are expected to have a low acute ecological impact (Hunger 2003). The results of empirical toxicity studies with both Disperse Blue 77 and several analogues are consistent with this expectation, indicating LC_{50} s on the 50 to 460 mg/L range. Although interpretation of results from these tests is complicated by the fact that these effect values are more than a thousandfold greater than the estimated solubility of the substance (i.e.,

approximately 0.01 mg/L), the data available do indicate that the aquatic toxicity of Disperse Blue 77 is low.

A range of aquatic toxicity predictions was also obtained from the various QSAR models considered for Disperse Blue 77 and its analogues. However, as for bioaccumulation, these QSAR ecotoxicity predictions for Disperse Blue 77 are not considered reliable because of the unique nature of disperse dyes, particularly structural and/or physical and chemical properties that fall outside of the models' domain of applicability.

The available empirical ecotoxicity information for Disperse Blue 77 (of which the reliability has yet to be verified) and results of available empirical aquatic toxicity data of analogues of Disperse Blue 77 indicate that it is not highly hazardous to aquatic organisms.

B - In Other Environmental Compartments

Due to its physical and chemical properties, there is a potential for Disperse Blue 77 to accumulate in sediment. Therefore, it would be desirable to obtain toxicity data for sediment-dwelling organisms. However, no ecological effects studies were found for this compound in media other than water.

Ecological Exposure Assessment

No data concerning concentrations of this substance in water in Canada have been identified. Environmental concentrations are, therefore, estimated from available information. Environment Canada's Industrial Generic Exposure Tool – Aquatic (IGETA) was used to estimate the (reasonable worst case) concentration of the substance in a generic watercourse receiving industrial effluents (Environment Canada 2008b). The generic scenario is designed to provide these estimates based on conservative assumptions regarding the amount of chemical processed and released, the number of processing days, the sewage treatment plant removal rate and the size of the receiving watercourse. The tool models an industrial-release scenario based on loading data from sources such as industrial surveys and knowledge of the distribution of industrial discharges in the country, and calculates a predicted environmental concentration (PEC). The equation and inputs used to calculate the PEC in the receiving watercourse are described in Environment Canada (2008b). The maximum mass of chemical used at a single facility is assumed to be the threshold reporting value of 1000 kg for the 2006 section 71 notices, a level that was not reached by any company. As a conservative estimate, handling and processing losses were assumed to be 20%. The receiving body information is highly conservative, assuming the chemical is released to a very small river without treatment. The conservative PEC for water was calculated to be 0.022 mg/L (Environment Canada 2008d).

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine various supporting information and develop conclusions based on a weight-of-evidence approach and using precaution as required under CEPA 1999. Particular consideration was given to risk quotient analysis, persistence, bioaccumulation, toxicity, sources and fate in the environment.

A predicted no-effect concentration (PNEC) was estimated based on the nominal lethal concentration (LC₅₀) to fish (*Pimephales promelas*). The 96-hour LC₅₀ for Disperse Blue 7 (CAS RN 3179-90-6), an analogue of Disperse Blue 77, was 52 mg/L (Table 7b). A factor of 100 was then applied to account for extrapolating from acute to chronic (long-term) toxicity and from laboratory results for one species to other potentially sensitive species in the field. The resulting PNEC is 0.52 mg/L. This value is close to the upper bound of the estimated range of solubility of the substance (0.2 mg/L; Table 2). When compared to the conservative PEC calculated for water above, the resulting conservative risk quotient (PEC/PNEC) is $0.022/0.52 = 0.042$. The calculated risk coefficient is less than one, therefore indicating a low potential for ecological harm resulting from local exposure to a point source industrial release to the aquatic environment associated with calculation of the PEC and PNEC. Given that a conservative estimate of exposure and risk was used, a more detailed evaluation of risk resulting from this type of source is not considered necessary.

Based on the available information, Disperse Blue 77 is expected to be persistent in water, soil and sediment; it is also expected to have a low bioaccumulation potential. The low importation volumes of Disperse Blue 77 into Canada, along with information on physical and chemical properties and its uses, indicate a low potential for releases into the Canadian environment. Once released into the environment, it will be found mainly in water, but will eventually transfer to sediment. It is also expected to have a low to moderate potential for inherent toxicity to aquatic organisms. Risk quotients for aquatic exposures indicate that Disperse Blue 77 concentrations likely do not exceed concentrations associated with harmful effects, even when using conservative scenarios and assumptions. Therefore Disperse Blue 77 is unlikely to be causing harm to populations of aquatic organisms in Canada.

Uncertainties in Evaluation of Ecological Risk

The persistence assessment is limited by the lack of experimental biodegradation data, which necessitated the generation of model predictions.

Uncertainties also exist because of the lack of information on environmental concentrations (e.g., monitoring data) in Canada for Disperse Blue 77. Uncertainties are also associated with the fraction of substance in commerce that is released, and with the fraction that is removed in sewage treatment plants. Consequently some conservative assumptions were made when using models to estimate concentrations near point sources.

Although that the total mass of the substance in commerce may have been underestimated - because of its unreported presence in down-the-drain consumer products imported into Canada – any releases associated with such uses would likely be spread over wide areas and the resulting exposure concentrations should be lower than those resulting from industrial releases and thus are also expected to pose little risk.

Regarding toxicity, based on the anticipated release pattern for the substance, the significance of sediment as a medium of exposure is not well addressed by the effects data available. Indeed, the only effects data identified apply primarily to pelagic aquatic exposures. An additional source of uncertainty relates to the fact that the toxic effects that are reported to occur at concentrations well above the estimated solubility of the substance.

There are uncertainties associated with the estimated physical and chemical properties of this substance (e.g. water solubility), which are based entirely on information for analogues.

For the exposure assessment, the predicted environmental concentration (PEC) accounts for concentrations in water only, so exposure through soils, suspended solids and sediments is not considered. However, given the current release scenarios and quantities used in Canada, overall environmental exposure is not likely to be significant at this time.

Conclusion

Based on the information presented in this screening assessment, it is concluded that Disperse Blue 77 is not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity, or that constitute or may constitute a danger to the environment on which life depends.

It is therefore concluded that Disperse Blue 77 does not meet the definition of toxic as set out in section 64 of CEPA 1999. Additionally, Disperse Blue 77 does not meet criteria for bioaccumulation potential but meets criteria for persistence as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

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Appendix 1. Robust study summary

Robust Study Summary Form: Aquatic B				
No	Item	Weight	Yes/No	Specify
1	Reference: Hu, Shuangqing and Shen, Genxiang (Environmental Testing Laboratory, Shanghai Academy of Environmental Sciences, Shanghai, China). 2008. Bioconcentration Test of C.I. Disperse Blue 77 in Fish. Prepared for Dystar in the name of Ecological and Toxicological Association of the Dyes and Organic Pigments Manufacturers (ETAD) Basel, Switzerland. Report No. S-071-2007. Submitted to Environment Canada on April 2008.			
2	Substance identity: CAS RN	n/a	Y	20241-76-3
3	Substance identity: chemical name(s)	n/a	Y	9,10-anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)-
4	Chemical composition of the substance	2	Y	
5	Chemical purity	1	N	
6	Persistence/stability of test substance in aquatic solution reported?	1	N	
7	If test material is radio-labelled, were precise position(s) of the labelled atom(s) and the percentage of radioactivity associated with impurities reported?	2		
Method				
8	Reference	1	Y	
9	OECD, EU, national, or other standard method?	3	Y	
10	Justification of the method/protocol if a non-standard method was used	2		
11	GLP (good laboratory practice)	3	N	
Test organism				
12	Organism identity: name	n/a	<u>Y</u>	zebra fish, <i>Brachydanio rerio</i>
13	Latin or both Latin and common names reported?	1	Y	
14	Life cycle age / stage of test organism	1	N	
15	Length and/or weight	1	Y	
16	Sex	1	N	
17	Number of organisms per replicate	1	Y	7
18	Organism loading rate	1	Y	
19	Food type and feeding periods during the acclimation period	1	Y	
Test design / conditions				
20	Experiment type (laboratory or field)	n/a	Y	Laboratory
21	Exposure pathways (food, water, both)	n/a	Y	Water
22	Exposure duration	n/a	Y	28 days
23	Number of replicates (including controls)	1	Y	
24	Concentrations	1	Y	20 mg/L
25	Food type/composition and feeding periods during the test	1	Y	
26	If BCF/BAF derived as a ratio of chemical concentration in the organism and in water, was experiment duration equal to or longer than the time required for the chemical concentrations to reach steady state?	3	Y	
27	If BCF/BAF derived as a ratio of chemical concentration in the organism and in water, were measured concentrations in both water and organism reported?	3	Y	

28	Were concentrations in the test water measured periodically?	1	Y	
29	Were the exposure media conditions relevant to the particular chemical reported? (e.g., for the metal toxicity - pH, DOC/TOC, water hardness, temperature)	3	Y	
30	Photoperiod and light intensity	1	Y	
31	Stock and test solution preparation	1	Y	
32	Analytical monitoring intervals	1	Y	
33	Statistical methods used	1	Y	
34	Was solubilizer/emulsifier used, if the chemical was unstable or poorly soluble?	n/a	N	
	Information relevant to the data quality			
35	Was the test organism relevant to the Canadian environment?	3	Y	
36	Were the test conditions (pH, temperature, DO, etc.) typical for the test organism?	1	Y	
37	Does system type and design (static, semi-static, flow-through; sealed or open; etc.) correspond to the substance's properties and the organism's nature/habits?	2	Y	
38	Was pH of the test water within the range typical for the Canadian environment (6 to 9)?	1	Y	
39	Was temperature of the test water within the range typical for the Canadian environment (5 to 27°C)?	1	Y	
40	Was lipid content (or lipid-normalized BAF/BCF) reported?	2	Y	
41	Were measured concentrations of a chemical in the test water below the chemical's water solubility?	3	N	
42	If radio-labelled test substance was used, was BCF determination based on the parent compound (i.e. not on total radio-labelled residues)?	3		
	Results			
43	Endpoints (BAF, BCF) and values	n/a	n/a	BCF
44	BAF or BCF determined as: 1) the ratio of chemical concentration in the organism and in water, or 2) the ratio of the chemical uptake and elimination rate constants	n/a	n/a	1
45	Whether BAF/BCF was derived from a 1) tissue sample or 2) whole organism?	n/a	n/a	2
46	Whether 1) average or 2) maximum BAF/BCF was used?	n/a	n/a	1
47	Score: ... %	79.2		
48	EC Reliability code:	2		
49	Reliability category (high, satisfactory, low):	Satisfactory Confidence		
50	Comments	<i>The present procedure is based on semi-static conditions (renewal of test solutions every 2 days). Therefore, test chemicals with very low water solubility like Disperse Blue 77, can also be characterized as to their bioconcentration potential without adding solvents or other auxiliary substances which may affect the results.</i>		