

Screening Assessment for the Challenge

**(Benzenesulfonamide, *N*-(4-amino-9,10-dihydro-3-methoxy-
9,10-dioxo-1-anthracenyl)-4-methyl-)
(Disperse Red 86)**

**Chemical Abstracts Service Registry Number
81-68-5**

**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 Benzenesulfonamide, *N*-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthracenyl)-4-methyl- (Disperse Red 86), Chemical Abstracts Service Registry Number 81-68-5. This substance was identified as a high priority for screening assessment and included in the Challenge because it was originally found to meet the ecological categorization criteria for persistence, bioaccumulation potential and inherent toxicity to non-human organisms, and it is believed to be in commerce in Canada.

The substance Disperse Red 86 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 Red 86 is a discrete organic substance that is used as a colorant (pigment, stain, dye, ink). The substance is not naturally produced in the environment. In 2006, between 1000 and 10 000 kg of Disperse Red 86 were imported, mainly in manufactured products and for application as a textile dye. The quantity of Disperse Red 86 imported into Canada and the nature of its uses suggest that it could be released into the Canadian environment.

Based on reported use patterns and certain assumptions, most of this substance (97%) is expected to end up in waste disposal sites, with the remainder being released to water. Disperse Red 86 is not soluble in water, is not volatile and is expected to be present in water mostly as small solid particles. For these reasons, Disperse Red 86 that is released to water is expected to ultimately settle to bed sediments. It is not expected to be significantly present in other media. As such, Disperse Red 86 is also not likely to be subject to long-range atmospheric transport.

Based on its physical and chemical properties, Disperse Red 86 does not degrade quickly in the environment and is therefore expected to be persistent in water, soil and sediments. Recent experimental data for an analogous substance suggest that Disperse Red 86 has a low potential to accumulate in the lipid tissues of aquatic organisms. The substance 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 Red 86 suggest that the substance is not highly hazardous to aquatic organisms.

No environmental monitoring data relating to the presence of Disperse Red 86 in the Canadian environment (air, water, soil, sediment) have been identified. For this screening assessment, a conservative exposure scenario was designed in which it is assumed that all industrial operations (users of the dye) discharge Disperse Red 86 into the same aquatic

environment. The predicted environmental concentration in water was below the predicted no-effect concentration calculated for sensitive aquatic organisms.

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 Red 86 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 Benzenesulfonamide, *N*-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthracenyl)-4-methyl- (Disperse Red 86) was identified as a high priority for assessment of ecological risk as it had been found to be persistent, bioaccumulative and inherently toxic to aquatic organisms and is believed to be in commerce in Canada. The Challenge for Disperse Red 86 was published in the *Canada Gazette* on August 18, 2007 (Canada 2007a). 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 pertaining to the uses of the substance were received.

Although Disperse Red 86 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, 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 May 2008. Key studies were critically evaluated; modelling results may have been used to reach conclusions. When available and relevant, information presented in hazard assessments 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.

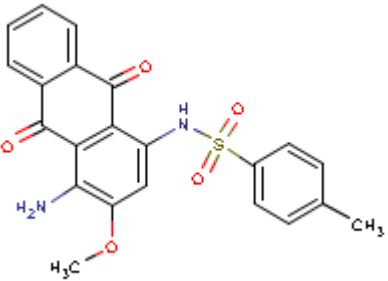
This screening assessment was prepared by staff in the Existing Substances Programs at Health Canada and Environment Canada and incorporates input from other programs within these departments. Additionally, a draft of this screening assessment was subject to a 60-day public comment period. While external comments were taken into consideration, the final content and outcome of the screening risk 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 screening assessment, this substance will be referred to as Disperse Red 86. Other names and identifying characteristics of this substance are presented in Table 1 below.

Table 1. Substance identity of Disperse Red 86

Chemical Abstracts Service Registry Number (CAS RN)	81-68-5
DSL name¹	<i>Benzenesulfonamide, N-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthracenyl)-4-methyl-</i>
National Chemical Inventories (NCI) names²	<i>Benzenesulfonamide, N-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthracenyl)-4-methyl-</i> (TSCA, AICS, PICCS, ASIA-PAC, NZIoC) <i>N-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthryl)-4-methylbenzenesulphonamide</i> (EINECS) <i>Disperse Red 86</i> (ENCs) <i>C.I. disperse red 086</i> (ECL) <i>C.I. DISPERSE RED 86</i> (PICCS)
Other names	<i>1-Amino-2-methoxy-4-p-tolylsulfonamidoanthraquinone</i> <i>Disperse Brilliant Pink FRL</i> <i>Eastman Polyester Pink R-LSH</i> <i>Eastman Polyester Pink RL</i> <i>Esterophile Light Pink R 3L</i> <i>Foron Brilliant Red SE 5GL</i> <i>N-(4-Amino-3-methoxy-1-anthraquinonyl)-p-toluenesulfonamide</i> <i>NSC 164933</i> <i>p-Toluenesulfonamide, N-(4-amino-3-methoxy-1-anthraquinonyl)-</i> <i>Serilene Pink G-LS</i> <i>Terasil Brilliant Pink 2GL</i> <i>Terasil Brilliant Red 2GLA</i> <i>Terasil Pink 2GLA</i> <i>Terasil Pink 2GLA01</i> <i>Teratop Pink 2GLA</i> <i>Viosperse Brilliant Pink 2GL-FS</i> <i>Viosperse Red 2G-LFS</i> <i>N-(4-Amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthryl)-4-methylbenzenesulfonamide</i>
Chemical group (DSL stream)	Discrete organics
Major chemical subclass	Anthraquinone
Chemical formula	$C_{22}H_{18}N_2O_5S$

Chemical structure	 <p>The image shows the chemical structure of Disperse Red 86. It consists of a central benzene ring substituted with a methylamino group (-NH₂), a methoxy group (-OCH₃), and a sulfonamide group (-NH-SO₂-C₆H₄-CH₃). This central ring is part of a larger anthraquinone-like system with two carbonyl groups (=O) and a phenyl ring attached to one of the carbonyl carbons.</p>
SMILES	<chem>O=C(c(c(C(=O)c1c(N)c(OC)cc2NS(=O)(=O)c(ccc(c3)C)c3)ccc4)c4)c12</chem>
Molecular mass	422.46 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); ENCS (Existing and New Chemical Substances); EINECS (European Inventory of Existing Chemical Substances); NZIoC (New Zealand Inventory of Chemicals); PICCS (Philippine Inventory of Chemicals and Chemical Substances); TSCA (Toxic Substances Control Act Chemical Substance Inventory).

Physical and Chemical Properties

It has been considered inappropriate to use predictive quantitative structure-activity relationship (QSAR) models to determine many physical and chemical properties of Disperse Red 86 and consequently data for chemical analogues as well as the read-across approach were used. The read-across values referred to all belong to the same chemical class as Disperse Red 86, namely disperse, anthraquinone dyes. However, chemical structures as well as CAS numbers were not available for substances in this class. When possible, ranges of values are given in order to give an approximation of the uncertainties.

Information on several disperse anthraquinone dyes was obtained from the following sources: Anliker et al. 1981, Anliker and Moser 1987, Baughman and Perenich 1988, ETAD 1992, ETAD 1995 and Brown 1992. These compounds have higher molecular weights (> 300 g/mol) and solid crystalline structures, decompose at temperatures 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 as they are designed to be so.

Table 2 contains analogue as well as read-across experimental and calculated physical and chemical properties of Disperse Red 86 that are relevant to its environmental fate.

Table 2. Physical and chemical properties for Disperse Red 86

Property	Type ¹	Value	Temperature (°C)	Reference
Melting point² (°C)	Read-across	225		Anliker and Moser 1987
		~130 to 330		Baughman and Perenich 1988
Boiling point³ (°C)	Not Applicable			
Density (kg/m ³)	Not available			
Vapour pressure (Pa)	Read-across	~2.7x10 ⁻¹¹ to 1.3x10 ⁻⁴ (2x10 ⁻¹³ to 1x10 ⁻⁶ mm Hg)	25	Baughman and Perenich 1988
Henry's Law constant (Pa·m ³ /mol)	Read-across ⁴	10 ⁻⁹ to 10 ⁻¹ (10 ⁻¹⁴ to 10 ⁻⁶ atm m ³ /mol)		Baughman and Perenich 1988
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 73	0.2 (2x10 ⁻⁴ g/L)		
	Analogue Disperse Blue 60	2 x 10 ⁻² (2 x 10 ⁻⁵ g/L) ⁷		
n-octanol solubility (mg/L)	Read-across	120	20	Anliker and Moser 1987
pK_a (Acid dissociation constant) (dimensionless)	Modelled	8.38		ACD/pK _a DB 2005

¹ These extrapolated values used for Disperse Red 86 are based on evidence on disperse dyes submitted to Environment Canada under the *New Substance Notification Regulations* (ETAD 1995) and the 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 Red 86.

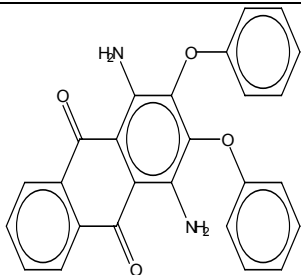
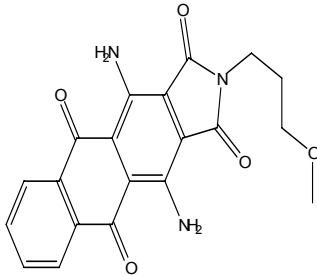
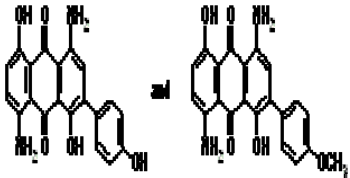
⁵ Log K_{ow} was obtained using the HPLC method.

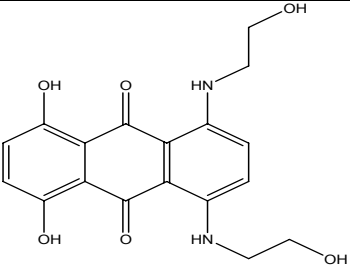
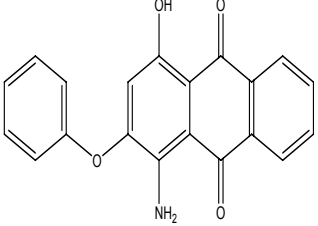
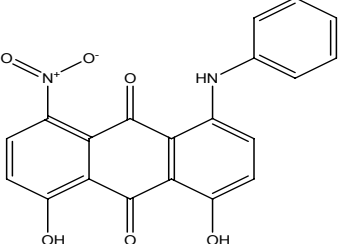
⁶ Log K_{oc} values are based on calculations by Baughman and Perenich (1988) using a range of measured solubilities for commercial dyes and an assumed melting point of 200°C.

⁷ Tested as active ingredient (FAT-36’152/C) and not as dispersion (ETAD 1992).

Structural disperse anthraquinone analogues to Disperse Red 86 are presented in Table 3a below. Certain physical and chemical properties (see Table 2), empirical bioaccumulation data (see Table 6) and empirical toxicity data (see Table 7) of these analogues were used in support of the weight of evidence. Specifically, physical and chemical properties were obtained for structural analogues: (i) Disperse Violet 26, (ii) Disperse Blue 60 and (iv) Disperse Blue 73. Empirical toxicity data were obtained for the following analogues: (i) Disperse Violet 26, (iii) Disperse Blue 73, (iv) Disperse Blue 7 and (v) Disperse Red 60. Finally, aquatic bioaccumulation data were available for the following analogue: (vi) Disperse Blue 77.

Table 3a. Structural analogues for Disperse Red 86

	CAS RN* or Colour index number**	Common name	DSL name ¹	Structure of analogue	Available empirical data
i.	6408-72-6*	Disperse Violet 26	9,10-Anthracenedione, 1,4-diamino-2,3-diphenoxy-		Log K_{ow} , water solubility, aquatic toxicity
ii.	61104**	Disperse Blue 60	1H-Naphth[2,3-f]isoindole-1,3,5,10(2H)-tetrone, 4,11-diamino-2-(3-methoxypropyl)-		Log K_{ow} , water solubility
iii.	63265**	Disperse Blue 73	Not available		Log K_{ow} , water solubility, aquatic toxicity

	CAS RN* or Colour index number**	Common name	DSL name ¹	Structure of analogue	Available empirical data
iv.	3179-90-6*	Disperse Blue 7	9,10-Anthracenedione, 1,4-dihydroxy-5,8-bis[(2-hydroxyethyl)amino]-		Aquatic toxicity
v.	17418-58-5*	Disperse Red 60	9,10-Anthracenedione, 1-amino-4-hydroxy-2-phenoxy-		Aquatic toxicity
vi.	20241-76-3*	Disperse Blue 77	9,10-Anthracenedione, 1,8-dihydroxy-4-nitro-5-(phenylamino)-		Aquatic bio-accumulation

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 and chemical, toxicological 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, there are unavoidable uncertainties which would not exist if it were possible to utilise empirical water solubility and a log K_{ow} specific to the substance Disperse Red 86.

Table 3b. Differences between structural analogues for Disperse Red 86

	Common name	Differences with Disperse Red 86
i.	Disperse Violet 26	Contains an extra phenolic ring attached to an oxygen atom. Contains an extra amine group.
ii.	Disperse Blue 60	Contains an extra penta-ring with two double-bond oxygens, a nitrogen atom and a 3-carbon chain with a COH ₃ attached.
iii.	Disperse Blue 73	Has 2 extra alcohol groups, 1 extra amine group and may have an extra OCH ₃ or OH group.
iv.	Disperse Blue 7	Contains two extra 2-carbon chain side groups that are attached to terminal hydroxyl groups. Has an extra hydroxyl groups attached to the three phenol rings. Lacks an OCH ₃ group.
v.	Disperse Red 60	Has an oxygen atom connecting phenol groups instead of NH ₂ and SO ₂ groups. Has an extra OH group. Lacks a CH ₃ group on the phenolic ring.
vi.	Disperse Blue 77	Contains 2 extra hydroxyl groups and a nitro group. Lacks CH ₃ group attached to the phenolic ring.

Sources

Disperse Red 86 is not naturally produced in the environment.

Recent information was collected through industry surveys conducted for the years 2005 and 2006 under a *Canada Gazette* notice issued pursuant to section 71 of CEPA 1999 (Canada 2006 and 2007b). This notice requested data on the Canadian manufacture, import and use of the substance. In addition, the Declaration of Non-Engagement and/or Stakeholder Interest form associated with this notice further invited any companies to identify themselves as stakeholders if they had an interest in a listed substance.

In 2006, three companies reported importing this substance, and collectively they imported between 1000 and 10 000 kg of the substance. No companies reported manufacturing Disperse Red 86 above the prescribed reporting threshold of 100 kg/year in Canada. 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. Three companies reported a stakeholder interest in this substance (Environment Canada 2007a).

In 2005, no companies reported manufacturing or importing Disperse Red 86 in quantities above the prescribed reporting threshold of 100 kg/year. However, two companies identified themselves as having a stakeholder interest in the substance.

It should be noted that additional amounts of Disperse Red 86 are likely entering Canada in imported products containing the dye that were not identified in the section 71 survey because they are imported unknowingly, or in quantities below the 100-kg reporting threshold for the survey.

In the United States, between 10 000 and 500 000 pounds (4.54 to 22.7 tonnes) of Disperse Red 86 were manufactured and/or imported annually in 1998 and 2002 (US EPA 2007). In Europe, Disperse Red 86 is a low production volume chemical (10 to 1000 tonnes produced or imported per year) (ESIS 2008). Disperse Red 86 was in use in Denmark and Sweden during 2000 to 2005 (SPIN 2007).

Uses

In 2006, the use pattern code “Colorant – pigment – stain – dye – ink” was given for Disperse Red 86, and one of the importing companies appears to be a wholesaler and distributor of chemicals. Additional use pattern codes were reported; however, these cannot be disclosed as they have 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: “Colorant - pigment/stain/dye/ink” and “Textile, Primary Manufacture.” In the United States, Disperse Red 86 is used in textile mill products (CDC 2007).

Releases to the Environment

Mass Flow Tool

To estimate potential release of the substance to the environment at different stages of its life cycle, the Mass Flow Tool was used (Environment Canada 2008a). 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. Assumptions and input parameters used in making these estimates are based on information obtained from a variety of sources including responses to regulatory surveys, Statistics Canada, manufacturers’ websites and technical databases. 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 increase toward the end of the life-cycle.

Table 4. Estimated releases and losses of Disperse Red 86 to environmental media, chemical transformation and transfer to waste management facilities, based on the Mass Flow Tool¹

Fate	Proportion of the mass (%) ¹	Major life cycle stage involved ²
Released to receiving media:		
Soil	0	n/a ³
Air	0.05	Service life of article, product waste disposal
Sewer ⁴	2.72	Industrial use
Chemically transformed	0	n/a
Transferred to waste disposal sites (e.g., landfill, incineration)	97.23	Product waste disposal

¹For Disperse Red 86, 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: OECD 2004a, OECD 2004b, and OECD 2006. 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.

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

³Not applicable.

⁴Wastewater before any form of treatment.

Results indicate that Disperse Red 86 can be expected to be found largely in waste disposal sites (97%), due to the eventual disposal of manufactured items containing it. Unless specific information on the rate or potential for release of the substance from landfills or incinerators is available, the Mass Flow Tool does not quantitatively account for releases to the environment from disposal. No such information has been identified for Disperse Red 86. It should be noted, however, that long-term releases from waste disposal sites may be possible.

It is estimated that about 3% of Disperse Red 86 may be released into water (sewer) due to non-dispersive industrial use of this product as a colorant for textiles, and 0.05% of Disperse Red 86 may be released into air following the service life of manufactured articles containing this substance. Finally, it is estimated that Disperse Red 86 will not be released into soil.

Based on the above, water (sewers) is the environmental medium receiving the greatest proportion of Disperse Red 86, as this substance is emitted during product manufacturing and processing. It is anticipated that the majority of the substance bound in the product will be sent to landfills for disposal.

Information regarding the use of Disperse Red 86 in manufactured items was received in response to the Section 71 survey and was used in the Mass Flow Tool to estimate potential releases to the environment. Although information on the total amount of Disperse Red 86 contained in manufactured items imported into Canada may not have been received, because losses from such items during their lifetime are expected to be relatively small, it is anticipated that the proportions of Disperse Red 86 that are released

to the various environmental media would not be significantly different from those estimated here.

Environmental Fate

As indicated by the results of the Mass Flow Tool (Table 4), the substance Disperse Red 86 is expected to be released to sewers during industrial processing and use. The relatively high pK_a of 8.38 indicates that dissolved forms of this substance will exist mostly in the neutral form at ambient pHs (6-8). The moderate to high $\log K_{ow}$ for analogues (3.3, 4.1, 5.1 and read-across > 4) and high analogue-based $\log K_{oc}$ (3.4 to 4.2) values (see Table 2) indicate that when in solution 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 the adsorption potential of solid crystalline dye structures is generally not well understood; therefore, the extent to which Disperse Red 86 is adsorbed to solids in the environment is uncertain.

Disperse Red 86 is a dense crystalline solid particle with a limited water solubility (see Table 2). 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 with uptake.

The rate of volatilization from water 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 indicate that Disperse Red 86 is essentially non-volatile. Therefore, loss of the substance to the atmosphere is not likely to be an important transport pathway from moist and dry soil surfaces as well as surface waters.

Finally, air is not considered to be an important medium for Disperse Red 86 due to the low volatility of this substance, as indicated by the low to negligible vapour pressure (2.7×10^{-11} to $1.3 \times 10^{-5} \text{ Pa}$, Table 2) and Henry's Law constant of its analogues. These data are consistent with the physical state (solid crystalline structure) of Disperse Red 86, which does not make it a likely candidate for volatilization or significant transport in air.

Persistence and Bioaccumulation Potential

Environmental Persistence

No experimental biological degradation data for Disperse Red 86 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 Red 86, there is no reason to suspect that biodegradation will be other than that described for dyes generally (ETAD 1995). As described below, modelled data in Table 5 support this assumption of non-degradability.

Given the expected release into waste water, persistence was primarily examined using predictive quantitative structure-activity relationship (QSAR) models for biodegradation in water. Because these degradation models are structure-based, their results are considered reliable since chemicals of structural comparability to Disperse Red 86 are contained in their training sets. Table 5 summarizes the results of available QSAR models for degradation in water. Disperse Red 86 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 Red 86

Model	Model and model basis	Result	Interpretation	Extrapolated half-life (days)	Extrapolation reference and/or source
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 1: Linear probability	0.51	Biodegrades fast	n/a ¹	
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 2: Non-linear probability	0.05	Does not biodegrade fast	n/a	
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 3: Expert Survey (ultimate biodegradation)	2.00	Months	60	US EPA 2002
				120	Aronson et al. 2006
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 4: Expert Survey (primary biodegradation)	3.10	Weeks	15	US EPA 2002; Aronson et al. 2006
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 5: MITI linear probability	-0.16	Does not biodegrade fast	> 60	Aronson et al. 2006
Biodegradation (aerobic)	BIOWIN 2000 Sub-model 6: MITI non-linear probability	0.00	Does not biodegrade fast	> 60	Aronson et al. 2006
Biodegradation (anaerobic)	BIOWIN 2000 Sub-model 7: Linear probability	-1.36	Does not biodegrade fast	n/a	

Model	Model and model basis	Result	Interpretation	Extrapolated half-life (days)	Extrapolation reference and/or source
Biodegradation	BIOWIN 2000 Overall Conclusion	no	Not ready biodegradable	n/a	
Biodegradation (aerobic)	TOPKAT 2004 Probability (MITI 1)	0	Persistent (< 0.3)	> 182	TOPKAT developers
Biodegradation (aerobic)	CATABOL c2004–2008 % BOD ² (OECD 301C)	6.3	Persistent (< 20%)	> 182	Calculated from BOD ² assuming first-order-rate kinetics

¹ Not available.

² Biochemical oxygen demand (BOD)

According to the results presented in Table 4, the majority of the probability models (BIOWIN 2, 5, 6 and 7) suggest this substance does not biodegrade rapidly. In fact, all probability results except those for BIOWIN 1 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 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 favourable anaerobic conditions, as indicated by the model BIOWIN 7. The overall conclusion from BIOWIN (2000) is that this substance is not readily biodegradable.

Other ultimate degradation models, CATABOL and TOPKAT, predict that Disperse Red 86 does not undergo any mineralization in a 28-day timeframe with the probability or extent of biodegradation in the range of very persistent chemicals. TOPKAT, which simulates the Japanese MITI 1 28-day biodegradation test, produced a probability of 0, which is less than the suggested cut-off for persistent substances in this model (< 0.3) (TOPKAT 2004). CATABOL predicted only 6.3% biodegradation based on the OECD 301 28-day ready biodegradation test (% BOD), which has been suggested to mean 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, TOPKAT 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 with this structure. Although it is possible that this substance will undergo faster primary degradation (based on results of BIOWIN 4), there are significant uncertainties (e.g., disperse 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 ratio 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 Red 86 meets the persistence criteria for water and soil (half-life in soil and water \geq 182 days) as well as sediments (half-life in sediments \geq 365 days) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential for Bioaccumulation

Bioaccumulation predictions as well as log K_{ow} estimates for Disperse Red 86 were obtained using predictive QSAR models; however, these results were considered unreliable as the available models are structure-based and do not account for the particulate nature of this substance. Since there are no specific experimental bioaccumulation studies for Disperse Red 86, available analogue and read-across data for disperse anthraquinone dyes were used in the weight of evidence for this section.

A recent empirical fish bioconcentration test for the substance Disperse Blue 77, a structural analogue of Disperse Red 86, was submitted to Environment Canada (Hu and Shen 2008). This test was performed according to OECD Guidelines for Testing of Chemicals, Test No. 305B-1996. The bioconcentration effect of Disperse Blue 77 to 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 the 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 determine the bioconcentrating capacity of the test substance on the test organisms. Samples from the test solutions and test organisms were taken daily from the 26th day to the last day during the exposure period. The lipid component was extracted from the test fish and the substance concentrations were measured in fish tissue and taken from the test solution. The measured concentrations of test substance, fish lipid content and BCF calculation are reported in Table 6a. Based on the measured concentrations in the exposure test medium and the test organism, the bioconcentration factor (BCF) of Disperse Blue 77 to Zebra fish was calculated as < 100.

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

		Sampling Time		
		26th day	27th day	28th 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 (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 study (2008) study has been reviewed and is considered acceptable (see Appendix 1). The reported BCF value of < 100 reflects the limited solubility of Disperse Blue 77 in both water and lipid extract and likely reflects the limit of detection in these media. Lack of detection in fish extracts (< 0.02 mg/L) suggests a limited solubility in lipids and/or partitioning behaviour in aqueous systems, more likely both. However, there is some uncertainty associated with limit bounded values in any study because the “true” value is not easily known. But given the structure and likely behaviour of this class of disperse dyes in aqueous systems, the BCF result is not unexpected. 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. While Disperse Red 86 contains some of these solubilizing functional groups (e.g., amino, sulphonamide), experimental solubility values for analogues containing many of the same groups remain quite low.

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, and it is expressed on the basis of wet body weight of the fishes (Anliker et al. 1981; Anliker and Moser 1987). A log K_{ow} of > 4 is also reported. The reason for the discrepancy between the high log K_{ow} and low log BCF 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 partitioning behaviour under BCF test conditions limits accumulation in fish lipids. It has also 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 much higher levels that may warrant conducting a fish accumulation test. The BCF study from Hu and Shen (2008) addresses this need.

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 $\log K_{ow}$ values for disperse anthraquinone-type dyes are > 4 , 5.1, 4.1 and 3.4 (Anliker et al. 1981; Anliker and Moser 1987; ETAD 1992 [see Table 2]). These values indicate that Disperse Red 86 may have the potential to bioaccumulate in organisms according to the $\log K_{ow}$ value alone. However, $\log K_{ow} > 4$ is likely a limit value (reflecting a limit of detection in water and thus there is an unknown upper limit of $\log K_{ow}$) while the $\log K_{ow}$ of 5.1 is nearly two log units (two orders of magnitude) higher than the $\log K_{ow}$ of 3.4 reported for another disperse anthraquinone dye. Additionally, the high $\log K_{ow}$ value of 5.1 may be questioned as it was experimentally derived using high-performance liquid chromatography (HPLC). HPLC is sometimes disputed as a method to derive $\log K_{ow}$ data, as it depends upon the relationship between the study 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 impossible. Without more detailed analytical information, it is difficult to ensure that this 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 methods. Thus, there is uncertainty with these data and it is difficult to determine bioaccumulation potential based solely on these results. The experimental details, the identities of the dyes as well as their corresponding Chemical Abstracts Service Registry Numbers (CAS RN) are not reported by Anliker et al. (1981) for both $\log K_{ow}$ and $\log BCF$ values. This lack of supporting information has also been noted by other authors (Baughman and Perenich 1988). This adversely affects the certainty of these data. However, as few bioaccumulation data have been identified for disperse anthraquinone dyes in general, these data were still considered for determining the bioaccumulation potential of Disperse Red 86. However, the uncertainty inherent in the Anliker et al. (1981) and Anliker and Moser (1987) data results in a lower weight given to these studies.

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 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. They also observed 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 Red 86 has a molecular weight of 409.42 g/mol (see Table 1) and its molecular structure is relatively uncomplicated; both these characteristics indicate a potentially significant bioaccumulation capability of this substance if molecular weight is used as the only parameter. In addition, an Environment Canada (2007c) report points out that there are no clear relationships for establishing strict molecular size cut-offs for assessing bioaccumulation potential. However, the report does not dispute the notion that a reduction in uptake rate can be associated with increasing cross-sectional diameter as demonstrated by Dimitrov et al. (2002, 2005). The maximum diameter of Disperse Red 86 and its conformers ranges from 13.7 to 18.9 Angstroms (1.37 to 1.89 nm) (BBM 2008) suggesting that a potential for a reduced uptake rate and in vivo bioavailability exists with this dye.

Considering the information discussed above, there is some uncertainty regarding the bioaccumulation potential of Disperse Red 86. Evidence is presented that both supports and argues against this substance having a significant bioaccumulation potential. However, greater reliability and thus weight has been assigned to the empirical BCF study from Hu and Shen (2008) as well as the potential for reduced uptake rate according to maximum cross-sectional diameter.

Although given lower weight due to lack of sufficient study details, the BCF results from Anliker et al. (1981) and Anliker and Moser (1987), also supports this conclusion. These data suggest a low bioaccumulation potential of Disperse Red 86. The only evidence for elevated bioaccumulation potential comes from two relatively high $\log K_{\text{ow}}$ values, 4.1 and 5.1, from two structural analogue substances and one unbounded $\log K_{\text{ow}}$ of > 4 value from Anliker (1981), which was also given a low weight when evaluating the significance of this evidence.

An additional, relatively lower $\log K_{\text{ow}}$ of 3.4 from another structural analogue also points to a conclusion that Disperse Red 86 has limited bioaccumulation potential. Therefore, when considering the overall weight of evidence, Disperse Red 86 is considered not to meet the bioaccumulation criteria (BCF, $\text{BAF} \geq 5000$) as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

Potential to Cause Ecological Harm

Ecological Effects Assessment

A - In the Aquatic Compartment

No experimental toxicity data for Disperse Red 86 were found. Aquatic toxicity predictions for this substance obtained using predictive QSAR models were considered unreliable and are not included in this screening assessment.

In general, due to their poor solubility in water (< 1 mg/L), disperse dyes have low acute ecological impact (Hunger 2003). In particular, acute toxicity to aquatic life forms is generally low.

In a study summary 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. The dyes were tested as a dispersion using a standard (non-toxic) dispersing agent. From the 11 disperse dyes tested by ETAD (1992), 3 are anthraquinone analogues of Disperse Red 86 (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 consideration in this screening assessment due to ambiguity in the reported values. Other empirical toxicity data were also obtained for two additional suitable anthraquinone dye analogues: Disperse Blue 7 and Disperse Red 60. Empirical aquatic toxicity data for Disperse Red 86 analogues are presented in Table 7 below.

Table 7. Empirical data for aquatic toxicity of Disperse Red 86 analogues

Common name	Test organism	Endpoint	Value (mg/L)	Reference
Disperse Violet 26	Zebra fish	96-hr LC ₅₀ ¹	> 500	ETAD 1992
	<i>Daphnia magna</i>	48-hr EC ₅₀ ²	> 200	
Disperse Blue 73	Zebra fish	96-hr LC ₅₀	> 500	
	<i>Daphnia magna</i>	48-hr EC ₅₀	200	
Disperse Blue 7	Fathead minnow (<i>Pimephales promelas</i>)	24-hr LC ₅₀	> 180	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>)	24-hr, 48-hr, 96-hr LC ₅₀	> 180	Little et al. 1974
		96-hr LC ₅₀	> 180	Little and Lamb 1973

¹ LC₅₀ – The concentration of a substance that is estimated to be lethal to 50% of the test organisms.

² EC₅₀ – The concentration of a substance that is estimated to cause some toxic sublethal effect on 50% of the test organisms.

The aquatic toxicity of Disperse Red 86 analogues presented in Table 7 ranged from moderate to low (acute LC₅₀/EC₅₀s from 52 to > 500 mg/L) based on tests performed for the duration of 24, 48 and 96 hours. All toxicity values exceeded 100 mg/L except one 96-hr

Fathead minnow LC₅₀ (52 mg/L). Although there are some differences in functional groups, the toxicity of Disperse Red 86 is expected to be comparable to that observed for these analogues due to overall similarity in molecular structure. Therefore, these aquatic toxicity values also suggest that Disperse Red 86 is not hazardous to aquatic organisms at relatively low concentrations (i.e., acute LC₅₀ > 1 mg/L).

It should be noted that the experimental details for the dyes Disperse Violet 26 and Disperse Blue 73 (ETAD 1992) were not provided, greatly limiting evaluation of these studies. Consequently, the results of these studies were given a lower weight. Also, it is important to note that all of the toxicity values presented exceed the solubility of the anthraquinone analogues presented in Table 2. This considerably complicates the interpretation of the toxicity results. In particular, it must be considered that different modes of action – one resulting from exposure to suspended particles and another to the dissolved substance – could be combining to cause the negative effects. However, despite these uncertainties these data were considered usable and are included in this screening assessment when evaluating the weight of evidence.

In conclusion, results of the available aquatic toxicity data for disperse anthraquinone dyes indicate that the substance Disperse Red 86 is not hazardous to aquatic organisms at low concentrations (i.e., acute LC₅₀ > 1.0 mg/L).

B - In Other Environmental Compartments

No effects studies for non-aquatic non-human organisms were found for this compound.

Ecological Exposure Assessment

No data concerning concentrations of this substance in water in Canada have been identified. As Disperse Red 86 is used in industrial facilities and can be released to water, Environment Canada's Industrial Generic Exposure Tool – Aquatic (IGETA) was employed to conservatively estimate a substance concentration in a generic water course 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 PEC for Disperse Red 86 was calculated based on a use quantity of 10 000 kg for a single facility (which is the upper limit of the range of the reported quantities imported into Canada in 2006). It was assumed that 3% of this quantity was lost to water during handling and processing (based on the Mass Flow Tool results presented in Table 3), that 0% was removed in an STP and that the STP discharged into a generic small river. The equation and inputs used to calculate the PEC in the receiving watercourse are described in Environment Canada (2008b).

The water PEC, resulting from industrial releases, is 0.0335 mg/L (Environment Canada 2008c).

Characterization of Ecological Risk

The approach taken in this ecological screening assessment was to examine available scientific information and develop conclusions based on a weight-of-evidence approach and precaution as required under CEPA 1999.

A predicted no-effect concentration (PNEC) was estimated based on the nominal lethal concentration (LC₅₀) to fish (*Pimephales promelas*). The 96-hr LC₅₀ for Disperse Blue 7 (CAS RN 3179-90-6), an analogue of Disperse Red 86, was 52 mg/L (see Table 6 above). A factor of 100 was then applied to account for uncertainty in extrapolating acute to chronic (long-term) toxicity, laboratory to field results, as well as uncertainty associated with using toxicity data for an analogue substance. The resulting PNEC is 0.52 mg/L. This value is close to the upper bound of the range of analogue-base water solubility estimated for this substance (0.02 – 0.2 mg/L; Table 2). When compared to the conservative PEC calculated above, the resulting risk quotient (PEC/PNEC) is $0.0335/0.52 = 0.0645$. The calculated risk coefficient is less than one, indicating that aquatic harm is unlikely. Given that IGETA provides a conservative estimate of exposure and risk, the results indicate a low potential for ecological harm resulting from local exposure to a point source industrial release to the aquatic environment.

Based on the available information, Disperse Red 86 is expected to be persistent in water, soil and sediment, but it is not expected to have a high bioaccumulation potential. The importation volumes of Disperse Red 86 into Canada, along with information on its uses, indicate a relatively 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 toxicity to aquatic organisms. Risk quotient for aquatic exposure indicates that Disperse Red 86 concentrations likely do not exceed concentrations associated with harmful effects, even when using conservative scenarios and assumptions. Therefore, Disperse Red 86 is unlikely to be causing harm to populations of aquatic organisms in Canada.

Uncertainties in Evaluation of Ecological Risk

Information on concentrations of Disperse Red 86 in the Canadian environment is lacking. Disperse Red 86 is used as a pigment/dyestuff in textile products and enters into Canada in manufactured items. It was imported into Canada in relatively low amounts (1000–10 000-kg range) in 2006 and it was not imported or manufactured in Canada in 2005. However, it is in commerce as a low production volume chemical in the United States and Europe. At present, Disperse Red 86 is not expected to be present at significant concentrations in the Canadian environment; however, uncertainties are associated with the fraction of substance in commerce as well as with the fractions that are released to sewers, and removed in sewage treatment plants. Consequently some

conservative assumptions were made when using models to estimate concentrations near industrial point sources.

Experimental data for ecotoxicity, degradation and bioaccumulation were not identified for Disperse Red 86. Persistence potential of this substance was estimated using predictive QSAR models. Although there are uncertainties associated with the use of QSAR models, results from the QSARs for biodegradation were consistent with other lines of evidence (e.g., empirical data indicating that analogous disperse dyes are resistant to degradation).

In contrast, the use of predictive QSARs was considered inappropriate to estimate physical and chemical properties, bioaccumulation potential and aquatic toxicity of this substance. Instead, studies for analogous disperse and anthraquinone dyes (read-across approach) were used to estimate these property values for Disperse Red 86. A number of scientific studies and reports used in this screening assessment are dated; however, more recent data on disperse anthraquinone dyes were not identified. In addition, experimental details, molecular structures as well as CAS numbers were not provided for some of the available studies for read-across substances and analogues, severely impeding evaluation of the studies' robustness.

In the exposure assessment, the predicted environmental concentration (PEC) accounts for concentrations in water only, so exposure through 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 Red 86 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 Red 86 does not meet the definition of "toxic" as set out in section 64 of CEPA 1999. Additionally, Disperse Red 86 meets the criteria for persistence but does not meet the criteria for bioaccumulation as set out in the *Persistence and Bioaccumulation Regulations* (Canada 2000).

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Appendix 1. Robust study summary

Robust Study Summaries Form and Instructions: 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 radiolabelled, 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 standard method was not used	2		
11	GLP (good laboratory practice)	3	N	
	Test organism			
12	Organism identity: name	n/a	Y	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 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 radiolabelled test substance was used, was BCF determination based on the parent compound (i.e. not on total radiolabelled 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 that may affect the results.</i>		