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DfE Alternatives Assessment for Nonylphenol Ethoxylates

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visit the DfE website at
http://www.epa.gov/dfe

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1. Introduction

A. Purpose and Scope

As part of its efforts to enhance public understanding and the safety of chemicals in commerce, EPA has taken steps to identify chemicals that may pose human and environmental health concerns and, in response, develop plans that consider potential regulatory and voluntary risk management actions. In August 2010, EPA released the Nonylphenol (NP) and Nonylphenol Ethoxylates (NPE) Action Plan[1] to address concerns over potential ecological and other effects from the manufacturing, processing, distribution in commerce, and uses of NP and NPEs. To implement part of the NP/NPE Action Plan, EPA's Design for the Environment (DfE) Program has prepared this Alternatives Assessment: *Alternatives for Nonylphenol Ethoxylates.*

DfE's Alternatives Assessment Program[2] helps industries choose safer chemicals and provides a basis for informed decision-making by developing a detailed comparison of potential human health and environmental effects of chemical alternatives. This Alternatives Assessment highlights and builds on the DfE Program's extensive work on surfactants and alternatives to NPEs, which includes development of the DfE Criteria for Safer Surfactants (U.S. EPA, 2011a); review of hundreds of surfactants in its Safer Product Labeling Program; sponsorship of an online database of safer surfactants (and other ingredients)—CleanGredients®; and creation, in partnership with EPA's Office of Science and Technology (in the Office of Water), of the Safer Detergents Stewardship Initiative (SDSI)[3]. Through SDSI, EPA recognizes product manufacturers who are formulating with safer surfactants in lieu of NPEs across entire product lines.

Over the years, DfE and other parts of EPA have conducted research to characterize NPEs and safer alternative surfactants. As a result, most of the information gathering, chemical profiling, and stakeholder interactions typical of an alternatives assessment have already taken place and serve as foundation and reference material for this document. To identify safer surfactants, DfE has worked in collaboration with diverse stakeholder groups, during both the development of the DfE Criteria for Safer Surfactants[4] and SDSI, which was launched at an EPA public meeting in June 2006. DfE routinely applies its safer surfactant criteria in evaluating products that are candidates to carry the DfE label and has researched and evaluated hundreds of surfactants, including the ones highlighted in this document. The methodology for this Alternatives Assessment reflects these substantial Agency investments. This report includes criteria that define safer NPE-alternative surfactants and lists a sampling of surfactants that meet the criteria.

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[1] The Nonylphenol and Nonylphenol Ethoxylates Action Plan is available at: http://www.epa.gov/oppt/existingchemicals/pubs/actionplans/RIN2070-ZA09_NP-NPEs%20Action%20Plan_Final_2010-08-09.pdf

[2] More information about DfE's Alternatives Assessment Program is available at: http://www.epa.gov/dfe/alternative_assessments.html

[3] More information about SDSI is available at: http://www.epa.gov/dfe/pubs/projects/formulat/sdsi.htm

[4] DfE's Criteria for Safer Surfactants is available at: http://www.epa.gov/dfe/pubs/projects/gfcp/index.htm#Surfactants

Also, the methodology in this Alternatives Assessment is tailored to the unique toxicological profile of surfactants and thus addresses a limited set of hazard endpoints. DfE focuses on the evaluation of NPE and its alternatives from an environmental health perspective, since the potential for toxicity to aquatic organisms—from the parent surfactant and its degradation byproducts—and environmental persistence have been important areas of toxicological research that have documented effects of concern.

The report for this Alternatives Assessment does the following:

- In Section 1B, recaps key points from the NP and NPE Action Plan (please see the Action Plan for more detailed information on NP/NPE production, uses, and discharges to the environment);

- In Section 2, illustrates the availability of safer NPE alternatives via DfE's hazard evaluation methodology: Table 2-3 presents the screening level environmental hazard summary for NPEs, followed by text explaining the hazard evaluation ratings;

- In Section 3, documents progress made in the adoption of safer surfactants, as well as opportunities for additional success; and

- In Section 4, lists all references cited in the document, by featured chemical.

B. Background on NP and NPEs

NPEs are surfactants, a functional class of chemicals that provide increased surface activity and reduce the surface tension of water, allowing easier spreading, wetting, and better mixing of liquids. Surfactants are classified into one of four categories based on their ionic properties in water: anionic (negative charge), nonionic (no charge), cationic (positive charge), and amphoteric (both positive and negative charges). NPEs are nonionic surfactants that are part of the broader category of surfactants known as alkyphenol ethoxylates (APEs). NPEs are considered "workhorse" surfactants given their cost-effectiveness and high performance in multiple applications.

The primary use of NP is as a raw material in the synthesis of NPEs. NPEs are manufactured by reacting NP with ethylene oxide (EO) under basic conditions, with the molar ratio of NP to EO determining the degree of ethoxylation (U.S. EPA, 2010a). NPE surfactants are referred to by their degree of ethoxylation; commercially available NPEs range from four moles of ethoxylates (NPE4) to 80 moles of ethoxylates (NPE80). NPEs with nine moles of ethoxylates (NPE9) are by far the most commonly manufactured NPE. While some CASRNs specific to certain levels of ethoxylates exist, all degrees of ethoxylation may be manufactured under the CASRN for poly-ethoxylates (CASRN 127087-87-0), as long as they are synthesized via polymerization reaction between NP and EO (U.S. EPA, 2010a).

NP and NPEs are produced in large volumes, with uses that lead to widespread release to the aquatic environment. NPEs represent approximately 80% to 85% of the volume of APEs (U.S. EPA, 2010a). U.S. and Canadian consumption of NPEs has been estimated between 300 and

400 million pounds per year (U.S. EPA, 2010a). NPEs are used in a wide variety of industrial and consumer applications, as shown in Table 1-1.

Table 1-1: Applications of NPE surfactants

- detergents
- cleaners
- degreasers
- dry cleaning aids
- petroleum dispersants
- emulsifiers
- wetting agents
- adhesives
- indoor pesticides
- cosmetics
- paper and textile processing formulations
- prewash spotters
- metalworking fluids
- oilfield chemicals
- paints and coatings
- dust control agents
- phosphate antioxidants for rubber and plastics
- miscellaneous uses, including lube oil additives

Source: (EPA 2010)

NPEs degrade to more toxic chemicals, including NP, which often partitions to sediment and accumulates (U.S. EPA, 2005a). The use of products containing NPE can result in the release of NP and other degradates to the environment, potentially exposing aquatic life to these compounds. NP is lethal to fish and other aquatic organisms at low concentrations (lower than for the parent NPE) in both acute and chronic fish studies (Talmage, 1994). In addition, effects on growth and reproduction have been documented (U.S. EPA, 2005a). The EPA recommended Aquatic Life Ambient Water Quality Criteria (AWQC) concentrations for NP are in the low parts per billion, based on this aquatic toxicity information. The EPA AWQC and its scientific basis are consistent with similar findings and regulatory actions taken by governments in Europe, Canada and Japan.

2. Evaluation of Alternatives to NPE Surfactants

A. Selection of Alternatives

Presented in Table 2-3 are nine alternatives to NPE surfactants, one from each of the major surfactant classes DfE has seen in its evaluation of detergent and cleaning products in its Safer Product Labeling Program. DfE selected the ten featured chemicals—NPE9, octylphenol ethoxylate (OPE)10 (a structural relative of NPE with a somewhat more hazardous profile), and the eight safer alternatives—as representative of its surfactant class and based on:

(1) the availability of an adequate dataset (i.e., sufficient experimental data to address all endpoints in the DfE Criteria for Safer Surfactants); and, except for NPE9 and OPE10,
(2a) frequent use in DfE-recognized formulations, and/or
(2b) inclusion on the CleanGredients® website of safer surfactant alternatives.

The chemicals presented are not intended as a comprehensive list of alternatives (note, for example, that the CleanGredients® database contains more than 300 surfactants), nor would all members of the structural classes represented by the featured alternatives necessarily meet the DfE Criteria for Safer Surfactants. Each potential NPE alternative must be evaluated on a case-by-case basis as to both its safety profile and functional characteristics. While each of the nine alternatives has the characteristics of a true surfactant (i.e., a hydrophobic, micelle forming head and a hydrophilic soil-removing tail), its ability to replace an NPE surfactant will depend on a formulation's performance demands.

Based on information from surfactant and cleaning product manufacturers who have partnered with DfE, the NPE alternatives are comparable in cost and performance, especially when viewed as part of a detergent system. Often, formulators will replace an NPE surfactant with a blend of two or more surfactants (e.g., a linear alcohol ethoxylate plus an alkyl glycoside). Depending on product type, a change in surfactant may also prompt other ingredient or formulary adjustments.

DfE chose NPE9 to represent the NPE class because it is the highest product volume NPE and the most commonly used in detergent products. Its hazard and biodegradation profile is typical of the NPE class.

B. Chemical Assessment Methodology

1. DfE Criteria for Safer Surfactants

As part of its Safer Product Labeling Program, DfE developed criteria for distinguishing safer from conventional chemicals within the functional component classes (e.g., surfactants, solvents, chelating agents) for cleaning products. A function-based approach makes it possible to identify distinguishing environmental and human health characteristics while maintaining ingredient performance and advancing safer chemistry. Only ingredients that meet DfE safer chemical criteria are allowed in DfE-labeled products. These criteria are used in this Alternatives Assessment of NPEs to show the foundation for DfE's surfactant assessments; the criteria developed for the Alternatives Assessment program (discussed in B.2.) enhance the basic assessments with chemical characterization detail. While the Criteria for Surfactants allow DfE to make pass-fail calls on a chemical's acceptability for use in DfE-labeled products, the Alternatives Assessment criteria permit assignment of hazard levels, e.g., a high, moderate or low hazard for persistence, and thus permit greater differentiation among surfactants.

The Criteria for Safer Surfactants (U.S. EPA, 2011a) use the following hazard characteristics to distinguish surfactants for cleaning products: the rate of aerobic biodegradation, hazard profiles of the degradation products, and degree of aquatic toxicity of the parent compound and degradation products. Since the surface active nature of surfactants causes toxicity to aquatic organisms, the criteria weigh these characteristics holistically and require that surfactants with higher aquatic toxicity demonstrate a faster rate of biodegradation without degradation to products of concern. Surfactants that meet the criteria are acceptable for use in a DfE-labeled cleaning product[5] (see Table 2-1) and reflect safer chemistry that can substitute for NPEs in general detergent uses.

[5] It is important to note that surfactants in products that typically by-pass sewage treatment must meet the more stringent thresholds in DfE's Criteria for Environmental Fate & Toxicity for Chemicals in Direct Release Products.

Table 2-1 Criteria for Safer Surfactants

Acute Aquatic Toxicity (L/E/IC50 Value)[1]	Rate of Biodegradation
≤1 ppm	May be acceptable if biodegradation[2] occurs within a 10-day window without degradates of concern[3]
>1 ppm and ≤10 ppm	Biodegradation[2] occurs within a 10-day window without degradates of concern[3]
>10 ppm	Biodegradation[2] occurs within 28 days without degradates of concern[3]

1. In general, there is a predictable relationship between acute aquatic toxicity and chronic aquatic toxicity for organic chemicals, i.e., chemicals that have high acute aquatic toxicity also have high chronic aquatic toxicity. Since acute aquatic toxicity data are more readily available, the DfE Criteria use these data to screen chemicals that may be toxic to aquatic life.
2. Generally, >60% mineralization (to CO_2 and water) in 28 days.
3. Degradates of concern are compounds with high acute aquatic toxicity (L/E/IC50 ≤ 10ppm) and a slow rate of biodegradation (greater than 28 days).

2. Alternatives Assessment Criteria for Surfactants

To enhance our understanding of the characteristics that distinguish safer from conventional surfactants, this Alternatives Assessment applies relevant environmental toxicity and fate elements taken from the DfE's Alternatives Assessment Criteria for Hazard Evaluation (U.S. EPA, 2011b). The alternatives assessment rating system (key elements of which are described below in Table 2-2) complements and expands on the DfE Criteria for Safer Surfactants. Under the alternatives assessment criteria, chemicals rating "high" or "very high" for aquatic toxicity would be acceptable for use in a DfE-labeled product only if they rate "very low" for persistence. Chemicals rating "moderate" (or "low") for aquatic toxicity would be acceptable only if they rate "low" or "very low" for persistence. Table 2-3 presents a screening level hazard profiles for NPE and nine alternatives and indicates which of these chemicals meet the DfE Criteria for Safer Surfactants.

a. Criteria Used to Assign Persistence and Hazard Levels

Table 2-2 lists the criteria that were used to interpret the data collected in this document. The criteria for environmental persistence and aquatic toxicity are taken from the DfE Alternatives Assessment Criteria for Hazard Evaluation. As detailed in the Alternatives Assessment Criteria, the values for aquatic toxicity were derived from the GHS (GHS, 2009), EPA Office of Pollution Prevention and Toxics' (OPPT) New Chemicals Program (U.S. EPA, 2005b) and OPPT's criteria for HPV chemical categorization (U.S. EPA, 2009). For environmental persistence, the criteria were derived from OPPT's New Chemicals Program (U.S. EPA, 2005b) and the DfE

The DfE Criteria for Environmental Fate & Toxicity for Chemicals in Direct Release Products is available at http://www.epa.gov/dfe/pubs/projects/gfcp/index.htm#Toxicity

Master Criteria (U.S. EPA, 2010b), and reflect OPPT policy on PBTs (U.S. EPA, 1999). The DfE Criteria for Safer Surfactants (U.S. EPA, 2011a) defines degradates of concern for surfactants and that definition is used again in Table 2-3.

Table 2-2: Criteria Used to Assign Aquatic Persistence and Hazard Levels

Persistence Level	Criteria
Very High	Half-life in water, soil, or sediment > 180 days or recalcitrant
High	Half-life in water, soil, or sediment 60-180 days
Moderate	Half-life in water, soil or sediment < 60 but ≥ 16 days
Low	Half-life in water, soil, or sediment < 16 days OR passes Ready Biodegradability test not including the 10-day window.
Very Low	Passes Ready Biodegradability test with the 10-day window.
Hazard Level	**Acute Aquatic Toxicity Criteria**
Very High	LC/EC50 is < 1 mg/L
High	LC/EC50 is 1-10 mg/L
Moderate	LC/EC50 is >10-100 mg/L
Low	LC/EC50 is >100 mg/L
Hazard Level	**Chronic Aquatic Toxicity Criteria**
Very High	NOEC/LOEC is < 0.1 mg/L
High	NOEC/LOEC is 0.1-1 mg/L
Moderate	NOEC/LOEC is >1 - 10 mg/L
Low	NOEC/LOEC is > 10 mg/L

b. Sources of Information on Toxicological and Environmental Endpoints

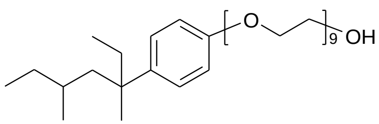
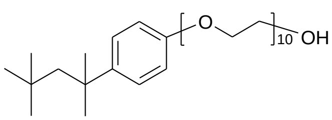
The chemical assessments in Table 2-3 combine primary and secondary data on the evaluated chemicals from six sources: (1) publicly available, measured (experimental) data obtained from a comprehensive literature review; (2) measured data from EPA OPPT confidential databases; (3) SAR-based estimations from the EPA New Chemical Program's Pollution Prevention (P2) Framework and Sustainable Futures predictive methods[6]; (4) estimations from the EPA Chemical Categories document, which groups chemicals with shared chemical functionality and toxicological properties into categories based on EPA's experience evaluating chemicals under the New Chemicals Program; (5) professional judgment of EPA staff who identified experimental data on closely related analogs; (6) confidential studies submitted by chemical manufacturers; and (7) the CleanGredients® database. When experimental data were lacking, Agency predictive models[7] and the expert judgment of scientists from EPA's New Chemical Program were used to assess physical/chemical properties, environmental fate, and aquatic toxicity endpoints.

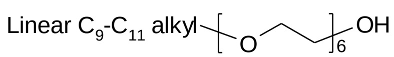
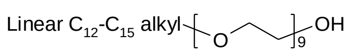
[6] The Sustainable Futures Initiative (SF) is available online at http://www.epa.gov/oppt/sf/

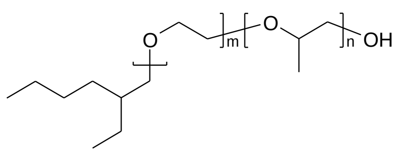
Table 2-3 Screening Level Environmental Hazard Summary for Surfactants

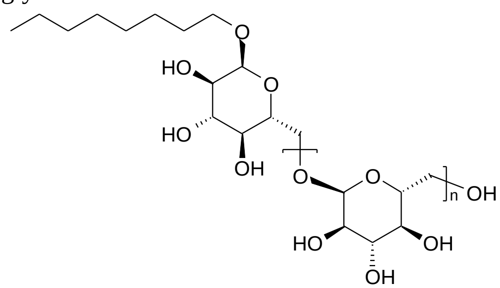
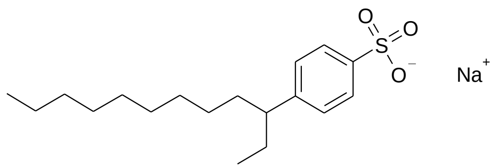
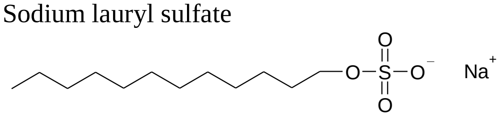
This table contains information on the inherent hazards of surfactant chemicals and indicates whether a chemical meets the DfE Criteria for Safer Surfactants. Evaluations are based on DfE's Criteria for Safer Surfactants and Alternatives Assessment Criteria. See http://www.epa.gov/dfe/pubs/projects/gfcp/index.htm#Surfactants and http://www.epa.gov/dfe/alternatives_assessment_criteria_hazard_eval_nov2010_final_draft2.pdf

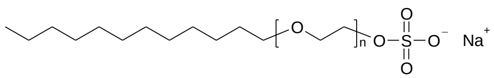
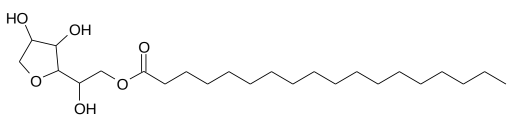
VL = Very low hazard L = Low hazard M = Moderate hazard H = High hazard VH = Very high hazard — Endpoints in colored text (VL, L, M, H, and VH) were assigned based on experimental data.
Endpoints in black italics (*VL, L, M, H,* and *VH*) were assigned using estimated values and professional judgment (Structure Activity Relationships).
Y=Yes…N=No

Chemical Class		**Fate**		**Aquatic toxicity[1]**				
Chemical	**CASRN**	**Persistence**	**Degradates of concern[2]**	**Acute**	**Chronic**	**Degradate Aquatic toxicity**	**Meets DfE Surfactant Criteria?**	**Synthesis**
Nonylphenol ethoxylates (NPEs)								
Nonylphenol ethoxylate (9EO); NPE9 	127087-87-0	**M**	**Y[3]**	**H**	**M**	**VH**	**N**	Nonylphenol is prepared from phenol and tripropylene, yielding a highly branched, predominantly para-substituted alkylphenol. Reaction of nonylphenol with ethylene oxide yields NPE surfactants.
Octylphenol ethoxylates (OPEs)								
Octylphenol ethoxylate (10EO); OPE10 	9036-19-5	**H[4]**	**Y[5]**	**H**	*H*	**VH**	**N**	Octylphenol is prepared from phenol and di-isobutylene, yielding a highly branched, predominantly para-substituted alkylphenol. Reaction of octylphenol with ethylene oxide yields OPE surfactants.

Chemical Class		Fate		Aquatic toxicity[1]				
Chemical	**CASRN**	**Persistence**	**Degradates of concern[2]**	**Acute**	**Chronic**	**Degradate Aquatic toxicity**	**Meets DfE Surfactant Criteria?**	**Synthesis**
Linear alcohol ethoxylates (LAE)								
C9-11 Alcohols, ethoxylated (6 EO) 	68439-46-3	**VL**	**N**	**H**	**H**	**L[6]**	**Y**	Linear alcohols, derived from fatty acids or alpha-olefins, are reacted with ethylene oxide to yield LAE surfactants. Many detergent grade LAEs make use of alcohols in the C10-C18 range.
C12-15 Alcohols, ethoxylated (9EO) 	68131-39-5	**VL**	**N**	**VH**	**H**	**L[6]**	**Y**	Linear alcohols, derived from fatty acids or alpha-olefins, are reacted with ethylene oxide to yield LAE surfactants. Many detergent grade LAEs make use of alcohols in the C10-C18 range.

Chemical Class			Fate		Aquatic toxicity[1]				
Chemical	CASRN		Persistence	Degradates of concern[2]	Acute	Chronic	Degradate Aquatic toxicity	Meets DfE Surfactant Criteria?	Synthesis
Ethoxylated/propoxylated alcohols									
Oxirane, methyl-, polymer with oxirane, mono(2-ethylhexyl ether); Ecosurf EH-9 	64366-70-7		**L**	**N**	**M**	*M*	**L**[6]	**Y**	2-Ethylhexanol is reacted with ethylene oxide and propylene oxide to yield this product. Other surfactants in this class use linear alcohols in place of 2-ethylhexanol.

Chemical Class		Fate		Aquatic toxicity[1]				
Chemical	CASRN	Persistence	Degradates of concern[2]	Acute	Chronic	Degradate Aquatic toxicity	Meets DfE Surfactant Criteria?	Synthesis
Alkyl polyglucose (APG)								
D-Glucopyranose, oligomeric, decyl octyl glycosides 	68515-73-1	VL	N	M	M	L[6]	Y	Fatty alcohols are reacted with glucose in the presence of an acid catalyst. Similar products may be prepared from other sugars, such as sucrose.
Linear alkylbenzene sulfonates (LAS)								
Benzenesulfonic acid, C10-13-alkyl derivs., sodium salt 	68411-30-3	VL	N	H	H	L[6]	Y	Benzene is alkylated with a linear olefin (either internal or terminal) in the presence of an acid catalyst, yielding a linear alkyl benzene (LAB). The LAB intermediate is sulfonated and neutralized to yield a linear alkyl benzene sulfonate surfactant.
Alkyl sulfate esters (AS)								
Sodium lauryl sulfate 	151-21-3	VL	N	H	H	L[6]	Y	Fatty alcohols are sulfated and neutralized to yield alkyl sulfate ester salts.

Chemical Class		Fate		Aquatic toxicity[1]				
Chemical	CASRN	Persistence	Degradates of concern[2]	Acute	Chronic	Degradate Aquatic toxicity	Meets DfE Surfactant Criteria?	Synthesis
Alkyl ether sulfates (AES)								
Polyoxy(1,2-ethanediyl), alpha-sulfo-omega-dodecyloxy-, sodium salt 	9004-82-4	L	N	H	H	L[6]	Y	Linear alcohol ethoxylates are sulfated and neutralized to yield alkyl ether sulfate salts.
Sorbitan esters								
Sorbitan monostearate 	1338-41-6	L[7]	N	H	H	L[6]	Y	Fatty acid methyl esters are reacted with sorbitan in the presence of a basic catalyst to yield sorbitan esters.

Note: Levels of 1,4-dioxane impurity in ethoxylated surfactants are limited to 100 ppm in the product formulation.
1. Acute toxicity data reviewed include 96-h LC_{50} assays in fish, 48-h EC_{50} or LC_{50} assays in invertebrates and 72-96-h EC_{50} assays in algae. Chronic toxicity values are not required for rating if adequate acute data are available.
2. Degradation products of concern for surfactants are compounds with high acute aquatic toxicity (L/E/IC50 $\leq$ 10ppm) and a slow rate of biodegradation (greater than 28 days).
3. One potential degradate, nonylphenol, raises concerns for its potential to affect the endocrine system.
4. Half-life cannot be reliably determined from the available biodegradation data for octylphenol ethoxylates. Based on biodegradation rate data, the time to achieve 50% degradation (as measured by oxygen demand) appears to be somewhat longer than 60 days.
5. One potential degradate, octylphenol, is more persistent and more toxic than the parent compound.
6. According to available biodegradation studies, this chemical ultimately degrades to CO_2, H_2O, and mineral salts, and therefore no aquatically toxic degradates are expected.
7. The available biodegradation data do not include information on the 10-day window.

c. Explanation of Hazard Evaluation Ratings

For each chemical in the summary matrix, the following explanatory text provides the basis for the hazard evaluation ratings and whether the chemical passes the DfE Criteria for Surfactants. Source materials with the data that support the evaluation ratings appear by chemical in Section 4.

NPE9 127087-87-0	
Persistence	MODERATE: Based on experimental data indicating that NPE9 does not pass standard ready biodegradability assays, reaching 31% in an OECD 30-day BOD test and 14-34% in an OECD modified Sturm test. (Kravetz, et al., 1991) Typical metabolites formed in aerobic biodegradation include nonylphenol and its lower-molecular weight ethoxylates (NPE1, NPE2) and ether-carboxylates (NPEC1, NPEC2). These have been found in STP effluents, sewage sludge and sediments, and can persist in the environment, especially under anaerobic conditions. (Naylor, 2004, pp. 432-436; Talmage, 1994, pp. 235-255; Ying, et al., 2002; Maguire, 1999; Bennie, 1999)
Acute Toxicity	HIGH: Based on experimental LC_{50} values for NPE9 in the range of 1.0-14 ppm in fish, EC_{50} values for NPE9 in the range of 2.9-14.0 ppm in daphnia and an EC_{50} value for NPE9 of 12 ppm in green algae. (Talmage, 1994, pp. 264-268; Talmage, 1994, pp. 271-275; Talmage, 1994, pp. 277-278, respectively)
Chronic Toxicity	MODERATE: Based on an experimental NOEC of 1.0 ppm in fish and a NOEC of 10 ppm in daphnia in 7-day growth assays with NPE9. (Talmage, 1994, pp. 282-283)
Degradate Toxicity	For nonylphenol: VERY HIGH: Based on experimental LC_{50} values in the range of 0.13-1.4 ppm in fish, EC_{50} values in the range of 0.14-0.47 ppm in daphnia and EC_{50} values in the range of 0.027-0.41 ppm in green algae measured for the degradate nonylphenol. (Talmage, 1994, pp. 264-268; Talmage, 1994, pp. 271-275; Talmage, 1994, pp. 277-278, respectively) In addition, a 33-day NOEC (survival) of 0.0074 ppm has been reported in fish and 21-day NOECs (growth, survival and sublethal effects) < 0.1 ppm have been reported in mysid shrimp for nonylphenol. (Talmage, 1994, pp 282-283)
DfE Criteria for Surfactants	**DOES NOT PASS**: Based on a classification of “High” for acute aquatic toxicity and “Moderate” for persistence, and the formation of persistent biodegradation products that are more toxic to aquatic organisms than the parent compound.

OPE10 9036-19-5	
Persistence	HIGH: Based on experimental biodegradation rate data, indicating that OPE10 reaches 10-53% biodegradation in 28 days in a shake-flask assay as measured by DOC removal, CO_2 evolution and BOD. (Talmage, 1994, pg. 351) Typical metabolites formed in aerobic biodegradation include octylphenol and its lower-molecular weight ethoxylates (OPE1, OPE2) and ether-carboxylates (OPEC-1, OPEC-2). (Naylor, 2004, pp. 432-436; Talmage, 1994, pp. 235-255)
Acute Toxicity	HIGH: Based on experimental LC_{50} values for OPE10 in the range of 8.9-12.0 ppm in fish (Talmage, 1994, pp. 264-268; Servos, 1999, pg. 141), an EC_{50} value for the analog OPE5 of 1.83 ppm in mysid shrimp (Talmage, 1994, pg. 273; Servos, 1999, pg. 141) and an EC_{50} value for OPE10 of 7.4 ppm in algae. (Servos, 1999, pg. 141)
Chronic Toxicity	HIGH: Based upon the experimental acute toxicity data and expert judgment. In the absence of data, chronic toxicity values for nonionic surfactants are estimated to be 10% of the measured acute toxicity data (LC/EC_{50} values).
Degradate Toxicity	For octylphenol: VERY HIGH: Based on experimental LC_{50} values for octylphenol in the range of 0.25- 0.29 ppm in fish, and experimental EC_{50} values for octylphenol in the range of 0.09-0.27 ppm in daphnia. (Servos, 1999, pg. 141; US EPA, 2009, pp 49-53) In addition, a 14-day NOEC of 0.084 ppm was measured in fish and a 21-day NOEC of 0.037 ppm (reproduction) was measured in daphnia. (Servos, 1999, pg. 140)
DfE Criteria for Surfactants	**DOES NOT PASS**: Based on a classification of "High" for acute aquatic toxicity and "High" for persistence, and the formation of persistent biodegradation products that are more toxic to aquatic organisms than the parent compound.

C_{9-11} Alcohols, ethoxylated (6EO) 68439-46-3	
Persistence	VERY LOW: Based on experimental data indicating that this compound passes standard ready biodegradation tests. C_{9-11}EO8 consumed 80% ThOD in 28 days in a closed bottle test, and C_{10-12} EO6 released 83% $ThCO_2$ in the OECD 301B assay. Persistent biodegradation products are not formed. C_{9-11}EO6 is also reported to pass several OECD 301-series tests, consistently meeting the 10-day window criterion. (HERA, 2009, pp. 28; Talmage, 1994, pp. 47-50, CleanGredients, 2011).
Acute Toxicity	HIGH: Based on experimental LC_{50} values ranging from 1.6-2 mg/L for C_{11}EO5 to 8-9 mg/L for C_{9-11}EO5 in fish; 5.4-14 mg/L for C_{9-11}EO6 in invertebrates; and 2.9-3.5 mg/L for C_{11}EO5 in algae (HERA, 2009, pp. 70, 76, 84, 86; Talmage, 1994, pp. 66, 71, 77).
Chronic Toxicity	HIGH: Based on an measured NOECs in juvenile fish of 1.0-4.4 mg/L (survival), 0.73 mg/L (reproduction) and 1.0 mg/L (growth) for C_{9-11} EO6; and a LOEC of > 2.0 mg/L in algae, measured in a 7-day reproduction study with C_{9-11}EO6 (Talmage, 1994, pp. 80, 95).
Degradate Toxicity	NOT EVALUATED: No persistent degradates are formed.
DfE Criteria for Surfactants	**PASS:** Based on a classification of "High" for acute toxicity and "Low" for persistence, with no formation of biodegradation products of concern.

C_{12-15} Alcohols, ethoxylated (9EO) 68131-39-5	
Persistence	VERY LOW: Based on experimental data indicating that this compound passes standard ready biodegradation tests. (Kravetz, et al., 1991). In addition, biodegradation information for C_{12-15} alcohols, ethoxylated (7EO and 9EO) are reported in the CleanGredients® Database indicating that these materials meet the 10-day window criterion in OECD 301-series tests. (CleanGredients, 2011) Persistent biodegradation products are not formed. (Talmage, 1994, pp. 47-50)
Acute Toxicity	VERY HIGH: Based on experimental LC_{50} values ranging from 1.2-11.0 ppm in fish, EC_{50} values ranging from 1.3-1.6 ppm in daphnia and an EC_{50} value of 0.70 ppm in green algae. (Talmage, 1994, pp. 61-67; Talmage, 1994, pg. 70; Talmage, 1994, pg. 77, respectively).
Chronic Toxicity	HIGH: Based on an experimental NOEC of 0.4 ppm in fish and an experimental NOEC of 1.0 ppm in daphnia, measured in 7-day growth assays with C_{12-15} alcohols, ethoxylated (EO9). (Talmage, 1994, pg. 79; Kravetz, et al. 1991)
Degradate Toxicity	NOT EVALUATED: No persistent degradates are formed.
DfE Criteria for Surfactants	**PASS:** Based on a classification of “Very high” for acute toxicity and “Very low” for persistence, with no formation of biodegradation products of concern.

Ecosurf EH-9 64366-70-6	
Persistence	LOW: Based upon experimental data indicating that this material achieves 60% or greater ThOD,/$ThCO_2$ ($\geq$ 70% DOC) biodegradation in an OECD 301F series assay, but without meeting the 10-day window criterion. (CleanGredients, 2011)
Acute Toxicity	MODERATE: Based upon an experimental 48-hr EC_{50} data of > 100 ppm in daphnia and a 72-hr EC_{50} in the range of 54-98 ppm in algae. (CleanGredients, 2011)
Chronic Toxicity	MODERATE: Based upon the experimental acute toxicity data and expert judgment. In the absence of data, chronic toxicity values for nonionic surfactants are estimated to be 10% of the measured acute toxicity data (LC/EC_{50} values).
Degradate Toxicity	NOT EVALUATED: No persistent degradates are formed.
DfE Criteria for Surfactants	**PASS**: Based on a classification of “Moderate” for acute toxicity and “Low” for persistence, with no formation of biodegradation products of concern. This surfactant is listed on CleanGredients® (CleanGredients, 2011)

D-Glucopyranose, oligomeric, decyl octyl glycosides 68515-73-1	
Persistence	VERY LOW: Based upon experimental data indicating that this material achieves 81-82% after 28-days in an OECD 301- D assay and 94% after 28 days in an OECD 301-E assay. This material met the 10-day window criterion in both tests. (Willing, et al., 2004, pg. 490)
Acute Toxicity	MODERATE: Based upon an experimental 96-hr LC_{50} of 101 ppm in fish, an experimental 48hr-EC_{50} of 20 ppm in daphnids and an experimental 72-hr EC_{50} of 47 mg/L in algae. (Willing, et al., pg. 498)
Chronic Toxicity	MODERATE: Based upon an experimental 72-hr NOEC of 5.7 mg/L in algae, and experimental data for an analog (C12-14 alkyl glycoside). Data reported for the analog include a 4-week NOEC of 1.8 mg/L in fish, a 21-day NOEC of 1.0 mg/L in daphnia and a 72-hr NOEC of 2.0 mg/L in algae. (Willing, et al., pg. 498)
Degradate Toxicity	NOT EVALUATED: No persistent degradates are formed.
DfE Criteria for Surfactants	**PASS**: Based on a classification of “Moderate” for acute toxicity and “Very low” for persistence, with no formation of biodegradation products of concern.

Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts 68411-30-3	
Persistence	VERY LOW: Based upon experimental data indicating that the $C_{10\text{-}13}$ alkyl derivative achieves 94% biodegradation in a DOC-Die away test, that the dodecyl alkyl derivative achieves 69% in an OECD 301-B test and that this compound ($C_{10\text{-}13}$ sodium salt) achieves 93-95% after 28 days in a DOC-Die away test that meets the 10-day window criterion (US EPA HPV, pp. 18-19, IUCLID pg. 25).
Acute Toxicity	HIGH: Based on experimental 96-hr LC_{50} values in the range of 1.7-7.8 ppm in fish (SIDS, 2005, pp. 175-182; HERA, 2009, pg. 24; Cavalli, 2004, pg. 396), 48-hr EC_{50} values in the range of 1.62-9.3 ppm in daphnia (SIDS, 2005, pp. 183-187; HERA, 2009, pg. 24; Cavalli, 2004, pg. 396) and 72-hr and 96-hr EC_{50} values in the range of 4.2-127 ppm for algae (SIDS, 2005, pp. 187-194; HERA, 2009, pg. 24).
Chronic Toxicity	HIGH: Based on experimental NOECs in the of 0.15-2.0 mg/L for 14-196-day chronic toxicity tests in fish (SIDS, 2005, pp. 201-206; HERA, 2009, pg. 25), experimental NOECs in the range of 0.3-3.25 mg/L in 21-day reproduction tests in daphnia (SIDS, 2005, pp. 211-212) and experimental NOECs of 0.1-3.1 mg/L for 72-hr and 15-day chronic toxicity tests in algae (SIDS, 2005, pp. 190-196, pp. 201-212).
Degradate Toxicity	NOT EVALUATED: No persistent degradates are formed.
DfE Criteria for Surfactants	**PASS**: Based on a classification of “High” for acute toxicity and “Very low” for persistence, with no formation of biodegradation products of concern.

Sodium lauryl sulfate 151-21-3	
Persistence	VERY LOW: Based upon experimental data indicating that this material achieves 60% or greater biodegradation as measured by oxygen uptake in assays similar to OECD 301C (MITI test) and meets the 10-day window criterion. (IUCLID, pp. 63-64)
Acute Toxicity	HIGH: Based on experimental LC_{50} values ranging from 1.0-34.9 ppm in fish, EC_{50} values ranging from 1.8-49 ppm in daphnia and EC_{50} values ranging from 30-150 ppm in green algae. (IUCLID, pp. 73-79; IUCLID, pp. 115-126; IUCLID, pp. 157-159, respectively).
Chronic Toxicity	HIGH: Based on an experimental NOEC of 0.75 ppm for blood effects in a 60-day chronic assay in fish (IUCLID, pg. 90), an experimental NOEC of 0.22 ppm in a 56-day chronic assay in invertebrates (Madsen, et al., 2001, pg. 21), and experimental NOEC values in the range of $\leq$ 0.1 – 50 ppm in 14-15-day chronic assays in green algae measuring cell count, growth rate and/or biomass. (IUCLID, pp. 151-152) Note that in the two assays reporting a NOEC of 0.1 or $\leq$ 0.1 ppm, the lowest dose tested was 0.1 ppm, and the effect (increase in cell count) was reported at 0.5 ppm. Madesn, et al. report a measured chronic NOEC of > 0.55 ppm for algae (Madsen, et al., 2001, pg. 21) and HERA reports a lowest chronic value for algae of 12 ppm (HERA,2002, pg. 22).
Degradate Toxicity	NOT EVALUATED: No persistent degradates are formed.
DfE Criteria for Surfactants	**PASS**: Based on a classification of “High” for acute toxicity and “Very low” for persistence, with no formation of biodegradation products of concern.

Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-dodecyloxy-, sodium salt 9004-82-4	
Persistence	LOW: Based on experimental data indicating that the $C_{12-14}AE_2S$ achieves 58-100% ThOD after 28 days in a Closed Bottle Test, that the $C_{12-18}AE_{8.5}S$ achieves 100% ThOD after 28 days in a Closed Bottle Test, and that this mixture corresponding to this CAS number achieves 58.6% degradation after 2 weeks in a MITI OECD 301-C test. Information on the 10-day window was not available, however, the MITI test data suggest that this compound could meet the 10-day window criterion. (Madsen, et al, 2001, pg. 25; National Institute of Technology and Evaluation, 2002).
Acute Toxicity	HIGH: Based on experimental 96-hr LC_{50} values in the range of 1.0-28 ppm in fish (Madsen, 2004, pg. 216; Madsen, et al., 2001, pg. 27), a 96-hr EC_{50} of 1.17 ppm in daphnia (Madsen, 2004, pg. 216) and an LC_{50} value of 4-65 ppm for C_{12-15} $AE_{1-3}S$ in algae (Madsen, 2004, pg. 216).
Chronic Toxicity	HIGH: Based on experimental NOECs ranging from 0.1-0.88 ppm in 20-30-day chronic toxicity tests in fish, NOECs ranging from 0.3-6.3 mg/L in 7-day chronic toxicity tests in daphnids, and NOECs ranging from 0.35-0.9 mg/L in 72-96-hour chronic toxicity tests in algae. (HERA,2002, pp. 18-20)
Degradate Toxicity	NOT EVALUATED: No persistent degradates are formed.
DfE Criteria for Surfactants	**PASS**: Based on a classification of “High” for acute toxicity and “Low” for persistence, with no formation of biodegradation products of concern.

Sorbitan monostearate 1338-41-6	
Persistence	LOW: Based on experimental data indicating that sorbitan monostearate achieves ≥ 75% biodegradation in 4 weeks as measured by BOD in the MITI test (OECD 301C). Information on the 10-day window was not available. (National Institute of Technology and Evaluation, 2002)
Acute Toxicity	HIGH: Based on an experimental LC_{50} value of > 6.3 ppm in fish, an EC_{50} value of >13 ppm in daphnia and an EC_{50} value of >56 ppm in green algae. (National Institute of Technology and Evaluation, 2002)
Chronic Toxicity	HIGH: Based on an experimental NOEC of 0.66 ppm in a 21-day reproduction study in daphnia. (National Institute of Technology and Evaluation, 2002)
Degradate Toxicity	NOT EVALUATED: No persistent degradates are formed.
DfE Criteria for Surfactants	**PASS**: Based on a classification of "High" for acute toxicity and "Low" for persistence, with no formation of biodegradation products of concern.

3. Activities to Promote the Use of Alternatives to NPE Surfactants

To complement the screening level hazard assessments presented in Section 2, this section highlights DfE activities that have led to significant progress in the adoption of safer surfactants, as well as opportunities for additional success. The brief descriptions below include links to more information.

DfE Safer Product Labeling and Criteria for Safer Surfactants

As part of its Safer Product Labeling Program, DfE developed Criteria for Safer Surfactants to supplement its Master Criteria for Safer Chemical Ingredients. DfE focuses its review of formulation ingredients on the distinguishing environmental and human health characteristics of chemicals within functional classes, including surfactants, solvents, chelating agents and fragrances. This approach allows formulators to use those ingredients with the lowest hazard in their functional class, while still formulating high-performing products. DfE has labeled more than 2,700 products, including a broad range of detergents and cleaning products, all of which contain surfactants that meet DfE's Criteria for Safer Surfactants (discussed within at Sec. 2.B.1). More information on the DfE labeling program, including a complete list of labeled product, is online at www.epa.gov/dfe.

The CleanGredients® Database

Safer surfactants are included in CleanGredients®, a database of safer cleaning product ingredients, online at www.cleangredients.org/home. The CleanGredients® database serves both as an ingredient resource for formulators seeking to make products that can carry the DfE label and as a marketplace for surfactant and other raw material suppliers interested in showcasing their safer, DfE-approved chemicals. The database contains over three hundred surfactant options in a variety of structural classes and lists key performance characteristics, like cloud point, critical micelle concentration, and specific gravity. The database also contains solvents, chelating agents and fragrances, which are used in cleaning and other product classes. Although CleanGredients® is foremost a resource for formulating safer cleaning products, it is also a resource for other product sectors that use these ingredient classes and are seeking safer substitutes. The database has the capacity to expand to other chemical classes and product categories.

The Safer Detergents Stewardship Initiative (SDSI)

Initiated by EPA in 2006, SDSI recognizes environmental leaders who voluntarily phase out or commit to phasing out the manufacture or use of NPE surfactants. SDSI complements EPA's AWQC for NP in reducing the load of toxic chemicals entering U.S. waters. Companies, such as chemical manufacturers, product formulators, retailers and distributors, institutional purchasers and others, are eligible to participate in SDSI. To date, DfE has awarded Champion status, its highest level of recognition, to more than 45 companies and Partner status to more than 20 companies. Through its work on SDSI and partnerships with industry and environmental advocates, DfE has identified alternatives to NPE surfactants that are comparable in cost, readily available, and which break down quickly to non-polluting compounds in fresh and salt water. For more information on SDSI, visit www.epa.gov/dfe/pubs/projects/formulat/sdsi.htm.

Having shown strong participation from cleaning product and detergent formulators, SDSI has the potential for similar results in other product classes. Especially of interest are products used outdoors where chemicals may be released directly to the environment (bypassing wastewater treatment); examples include de-icers, oilfield chemicals, dispersants, and dust control agents. SDSI may also serve as a model for other voluntary initiatives seeking to encourage a move from chemicals of potential concerns to safer alternatives.

Laundry Industry Phase-out of NPEs

For many years, the uniform and textile rental industry relied heavily on NPEs as the workhorse surfactants for Industrial/Institutional (I/I) laundry operations. The industry maintained that NPEs could not be replaced in their detergent formulations; they maintained that no other surfactants could match NPEs in performance, affordability or efficiency. Gradually, however, as surfactant manufacturers innovated to meet market demand for high-performing, more environmentally friendly alternatives, built their supply capacity, and lowered prices, I/I detergent formulators embraced the safer chemistry options. In response to the SDSI and the new market conditions, the I/I laundry industry has pledged to eliminate the use of NPE surfactants and is well along the way to reaching its phase-out goals. The current deadline for complete phase-out in all liquid detergents is December 31, 2013, and in all powder detergents, December 31, 2014.[7]

[7] As per letter from Charles Sewell, Vice President, Textile Rental Services Association of America to Lisa Jackson, Administrator, US EPA, June 22, 2010.

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