A proposed category approach on Exxal™ alcohol derivatives for evaluation to meet Safer Choice Direct Release Surfactant Criteria

Executive Summary

Safer choice direct release surfactants meet enhanced environmental criteria to address the potential for immediate contact with aquatic life. These criteria are outlined by the EPA[1]. ExxonMobil has engaged in an extensive in-house environmental testing strategy for ethoxylated derivatives of our Exxal™ alcohols in order to provide detailed characterization of their environmental profiles and support customers of these products in a wide range of applications. Where test data does not exist, our environmental toxicologists have developed sophisticated models and weight of evidence strategies to predict a range of environmental properties (including biodegradability and ecotoxicological hazard) of these substances.

Based on their environmental properties Exxal alcohol-based ethoxylated surfactants within specific ethoxylation ranges meet EPA Safer Choice Direct Release Criteria.

Given modeling, existing test data, and well-established structure activity relationships ExxonMobil proposes that the following ethoxylated derivatives (EO) will meet EPA criteria. The acceptability of the proposed categories are currently under review by the Safer Choice Program:

Exxal™ 8 with 20EO to 4EO meets the criteria and potentially down to 1EO.

Exxal™ 9 with 20EO to 7EO meets the criteria and potentially down to 3EO.

Exxal™ 10 with 20EO to 9EO meets the criteria and potentially down to 5EO.

Exxal™ 11 with 20EO to 7EO meets the criteria and potentially down to 6EO.

Exxal™ 13 with 20EO to 12EO meets the criteria and potentially down to 11EO.

Of interest, an ethoxylated surfactant using a naming convention tied to Exxal™ 13 (Alcohols, C11-14-iso-, C13-rich, ethoxylated CAS# 78330-21-9) is already listed on Safer Chemical Ingredients List (SCIL).

[1] https://www.epa.gov/saferchoice/standard#directrelease

High level overview of data which supports Exxal™ alcohol ethoxylated derivatives meet current Safer Choice Direct Release Criteria[2]

Variations in carbon chain lengths, numbers of ethoxyl (EO) units, and degree of branching can impact the performance and environmental properties of alcohol ethoxylate (AEO) surfactants. Ideal molecules for safer choice designation should be highly degradable with low aquatic toxicity. While exhaustive data sets are not available for all homologues or AEO mixtures, structure activity relationships (SARs) have been developed previously which can accurately predict these properties. (Table 1).

Table 1 – Structure activity relationship for key attributes of ethoxylated alcohols and environmental properties.

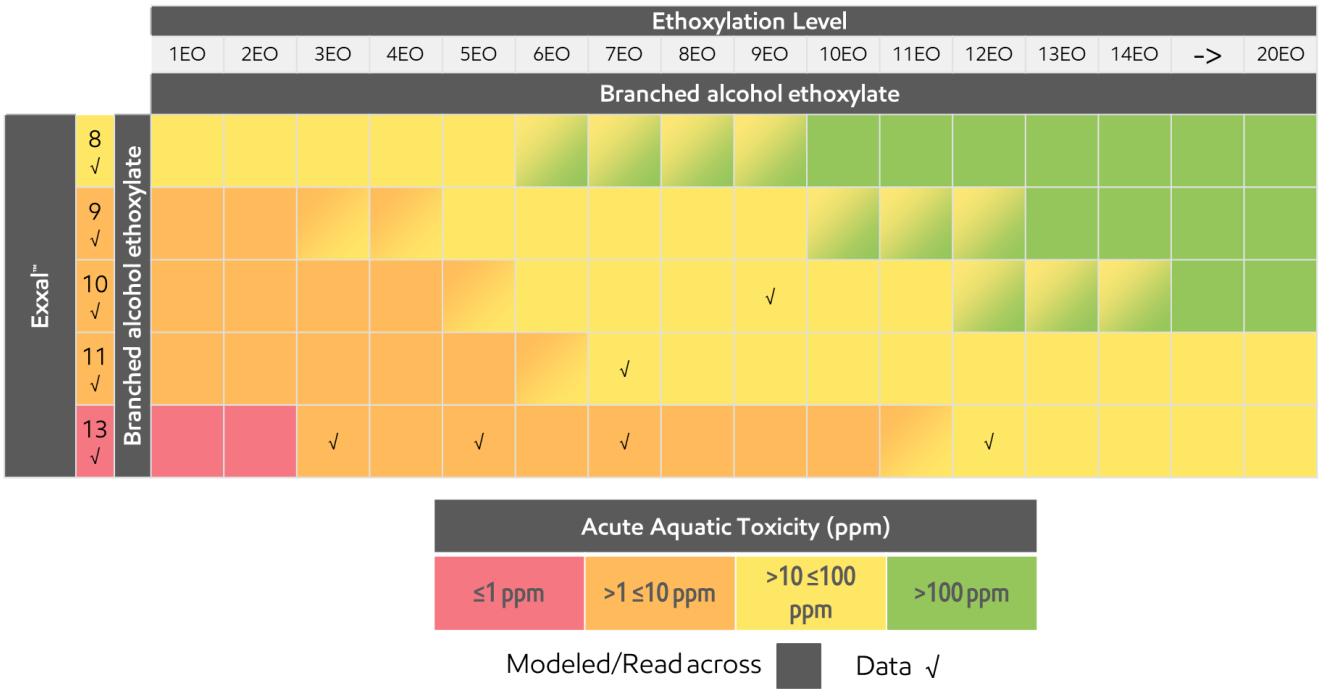
Property	Model	Output	Reference
Biodegradability	BioWIN v4.10 (BioWin 1-7, RBD Prediction)	Ready Biodegradability (Categorical)	US EPA, 2020
	Catalogic v.5.11 (301F Kinetic Model)	Ready Biodegradability (Quantitative) Primary Half-Lives (water)	Dimitrov et al., 2011
Aquatic Toxicity	Target Lipid Model (TLM)	L/EC50 and ChV (fish, invertebrates, algae)	Di Toro et al. 2000a,b; Bragin et al., 2019*
	ECOSAR v2.0	L/EC50 and ChV (fish, invertebrates, algae)	US EPA, 2020
Bioaccumulation	BCFBAF (Arnot-Gobas Upper Trophic BCF/BAF)	BCF and BAF (low, mid, upper trophic aquatic organisms incl. metabolism)	US EPA, 2020
	BCF Regression	BCF (fish; no metabolism)	

*Application of TLM specifically for alcohol ethoxylates.

Combining known structure activity relationships with existing data and knowledge of chemical structure, mechanism, and effects, one can develop a weight of evidence approach for filling data gaps and make informed decisions as to the environmental properties of a broad range of AEO products.

[2] Final determination is subject to EPA approval

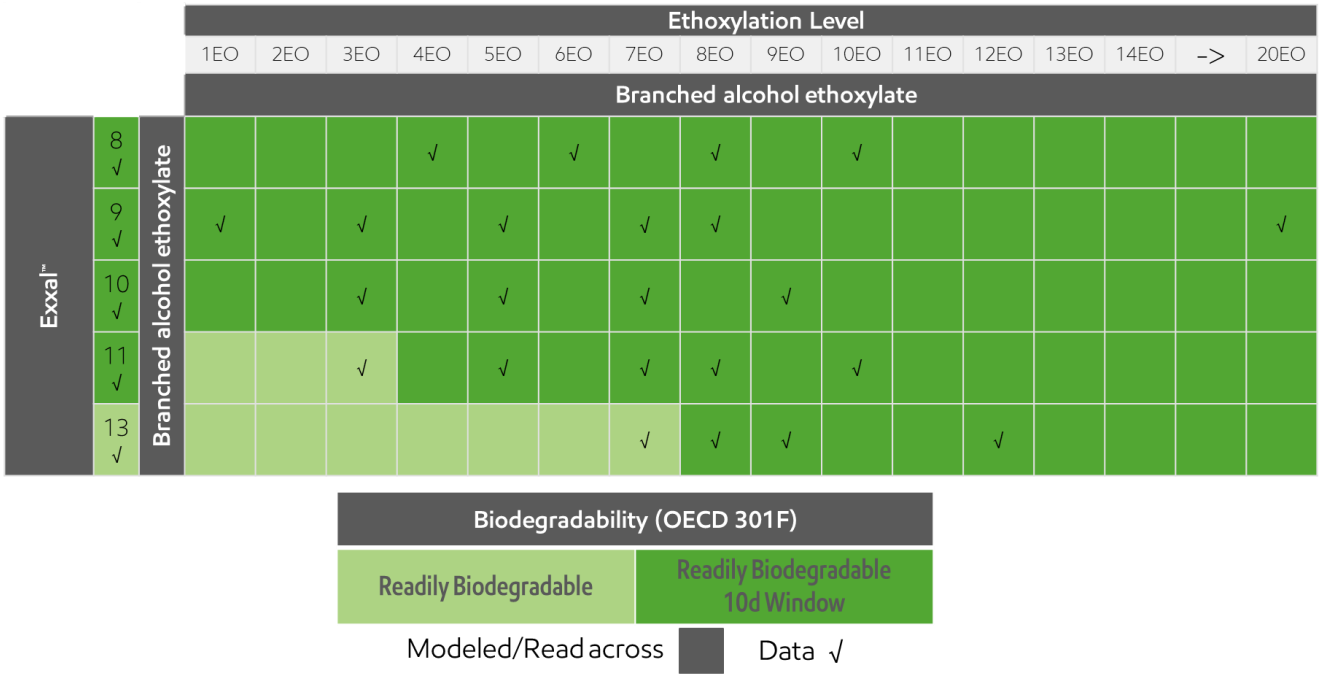
Table 2 – Acute toxicity profile of Exxal™ Alcohols ethoxylates from 1EO to 20EO



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 Safer Choice Criteria use these data to screen chemicals that may be toxic to aquatic life (see Sections 5.9 and 6.8 of the Safer Choice Master Criteria for Safer Ingredients). Per verbal guidance from relevant EPA staff, chronic data are not an absolute requirement and commonly, chronic toxicity is estimated to be acute/10. By applying this rule it is estimated that substances with >10 ppm for acute aquatic toxicity will pass the >1ppm threshold for chronic toxicity. This assumption is quite conservative, as significant work has been done to establish acute to chronic ratios (ACRs) for neutral organic chemicals (ACR = 5.22), whose domain includes AEO parent alcohols (Di Toro et al., 2000a,b; McGrath et al., 2009; Redman et al., 2012; Redman et al., 2017; McGrath et al., 2018). Recently this has been demonstrated to conservatively predict the chronic toxicity of alcohol ethoxylates (AEOs), specifically (Bragin et al., 2019).

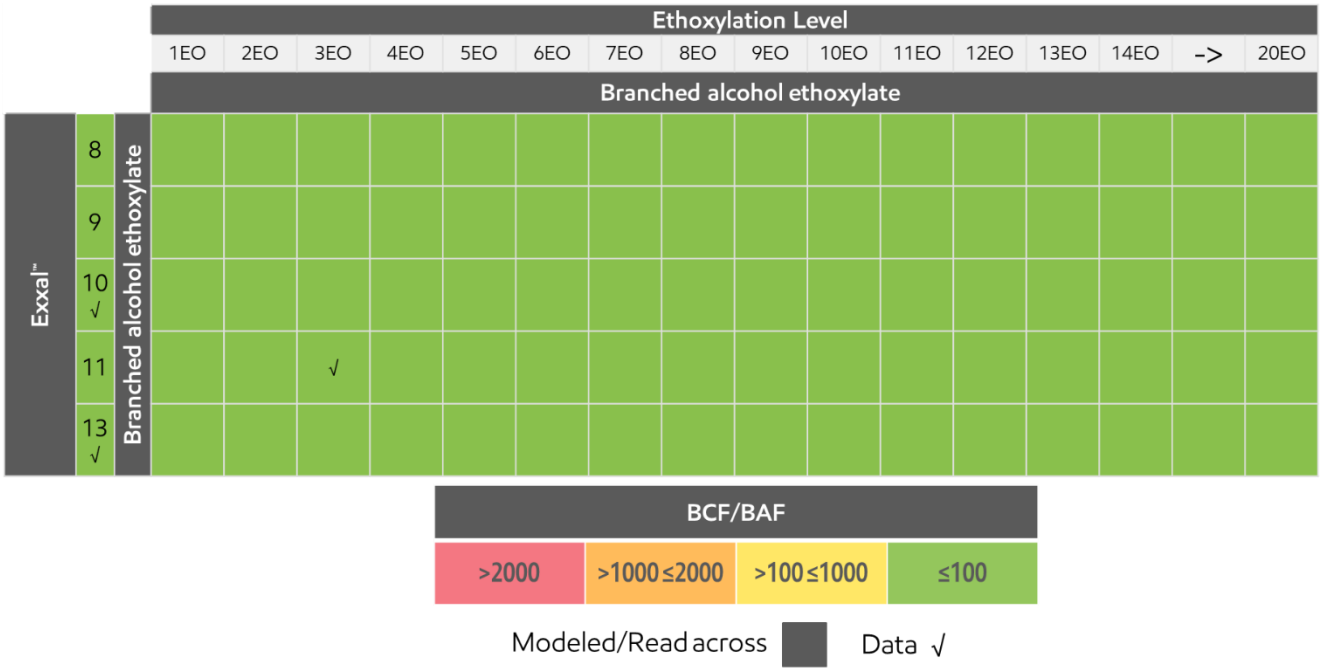
The biodegradability profile of our branched AEOs is well supported by a broad range of substance specific biodegradation testing (Bragin et al., 2019).

Table 3 – Biodegradation profile of Exxal™ Alcohols ethoxylates from 1EO to 20EO



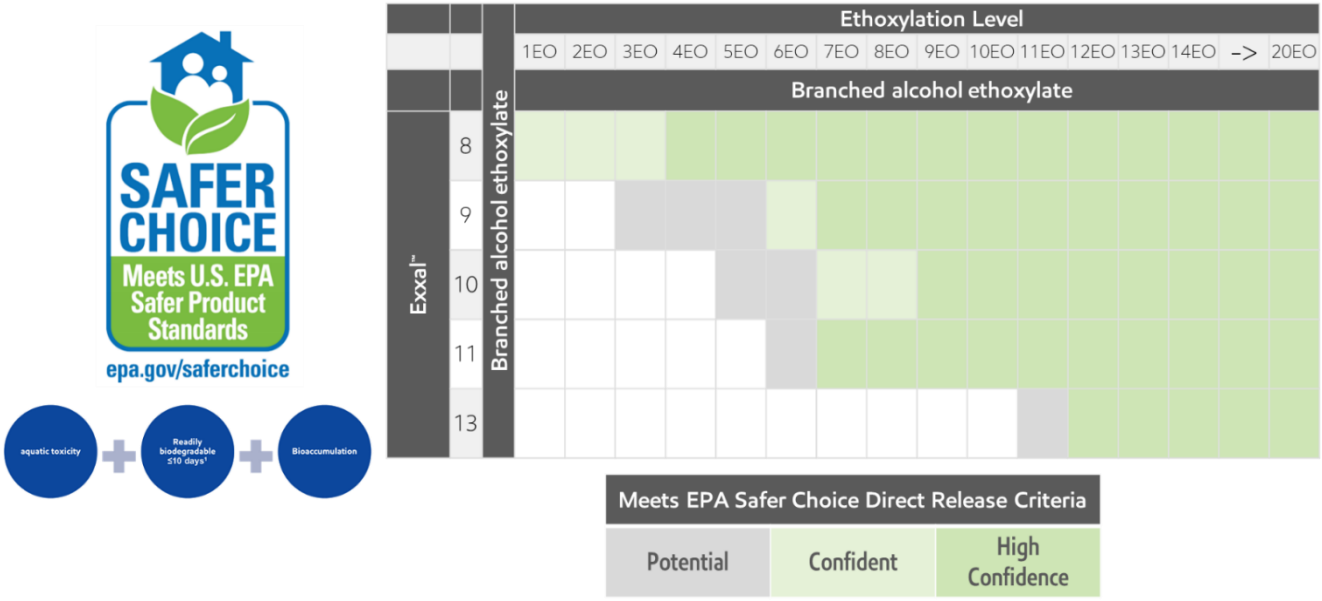
BCF data (Camenzuli et al., 2019) for several iso-branched parent alcohols (C10, 12, and 13) as well as BMF data (Gobas et al., 2020) for iso-branched C10 and C13 alcohols and a branched C11-3EO ethoxylate have been generated. BCF and BMF values for these substances are very low (5% lipid-normalized BCF range from 12 – 77 L/kg-ww for the parent alcohols, BMF values range from 0.001 – 0.003 for the parent alcohols and the C11-3EO ethoxylate) and support previous work which demonstrate low bioaccumulation potential and rapid metabolism of AEOs in aquatic organisms (Tolls et al., 2000 and Belanger et al., 2009). Further, BCF QSARs are in good agreement for alcohol ethoxylates and their parent alcohols, predicting low potential for bioaccumulation (Arnot & Gobas, 2003; Arnot & Gobas 2006). While the Safer Choice criteria does not explicitly consider BMF data, this information should be considered an additional higher-tier line of evidence to support low bioaccumulation/bioconcentration potential for poorly soluble or highly hydrophobic compounds for which the dietary route of exposure may be considered important (Gobas et al., 2020). These independent lines of evidence strongly support a weight of evidence conclusion for low bioaccumulation potential of AEOs in the aquatic environment.

Table 4 – Bio-concentration factor (BCF)/Bio-accumulation factor (BAF) for Exxal™ Alcohols ethoxylates from 1EO to 20EO



Compiling these pieces of information gives the following predictions for meeting EPA safer choice direct release criteria.

Table 5 – Range of Exxal™ Alcohols ethoxylates predicted to meet Safer Choice Direct criteria and level of confidence.



1. No degradation products of concern are compounds with high acute or chronic aquatic toxicity (L/E/IC50 ≤ 10ppm or LOEC ≤1 ppm) and a slow rate of biodegradation (greater than 28 days).

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