Environmental Fate and Ecotoxicity Endpoints for Nafol 22+

Nafol 22+ is distillation residues of a by-product of the C20 alcohols manufacturing process. It is a UVCB substance that comprises predominantly docosan-1-ol (C22), tetracosan-1-ol (C24), hexacosan-1-ol (C26) and eicosan-1-ol (C20). Together, these substances make up over 80% of the composition of olefines polymer, oxidized, hydrolyzed, distillation residues. The endpoints summarized below for biodegradability and ecotoxicity are from the registered Nafol 22+ data in REACH. They are based on the measured or estimated endpoints for the major constituents of Nafol 22+ using Category Approach (read-across) in a conservative manner in which the most sensitive study result from the constituent of the category was used. This is consistent with the Category Approach applied for Long Chain Alcohols (LCA) under REACH (Ref 21). The structure of the Category is associated with a consistency and predictability in the physicochemical, environmental, and ecotoxicological property data across its members because of the similarity in chemical structure of the members. In addition, certain branched and unsaturated structures are considered to have such similar properties that their inclusion in the category is well justified. Therefore, this read-across approach applies to the physicochemical, environmental fate, and ecotoxicity properties of this substance.

1. Biodegradability
   Two tests were conducted in accordance with OECD Guideline 301B (Ref 20-1, Ref 20-2, Ref 24). For Ref 20-1 and Ref 20-2, only the robust study summary (RSS) of the study is available. The test substance for Ref 20-1 was icosan-1-ol. There was 88.4% degradation at the end of the tests (28 days) and the test substances also achieved 60% degradation within the 10-day window. The test substance for Ref 20-2 was docosan-1-ol. There was 87.9% degradation at the end of the tests (28 days) and the test substances also achieved 60% degradation within the 10-day window. For Ref 24, the test substance was docosan-1-ol. There was 87.5% degradation at the end of the tests (28 days) and the test substances also achieved 60% degradation within the 10-day window. It is expected that Nafol 22+ is also readily biodegradable.

2. Hydrolysis
   This substance has no hydrolysable structural features and would be expected to be stable in water. Oxidation would not be expected under normal and relevant environmental conditions.

3. Adsorption/desorption
   The K_{oc} value was previously estimated using the SRC PCKOCWIN method, with the estimated K_{oc} values being 43,800 for 1-eicosanol and 149,000 for 1-docosanol (page 45, Ref 21). The SRC PCKOCWIN module has been replaced by KOCWIN in the current EPISUITE model (v4.11). Therefore, these K_{oc} values were further updated using the current KOCWIN and the updated logKow value of 8.3 (Ref 16). The estimated K_{oc} values for 1-eicosanol ranged from 51,380 to 127,200 L/kg (page 8, Ref 26-1). The estimated K_{oc} values for 1-docosanol ranged from 127,200 to 170,700 L/kg (page 8, Ref 26-2). The model input and output files are also included (Ref 26-1, Ref 26-2).

4. Bioaccumulation in aquatic specie

The bioconcentration factor (BCF) was calculated using the parabolic equation by Connell and Hawker (Ref 43). This approach is in accordance with standard EU recommendations. The calculated BCF was 31,800 for both 1-eicosanol and 1-docosanol (Ref 36).

5. Short-term toxicity to fish
   The measured/predicted (read-across) short-term toxicity to fish is as follows:
   a). icosan-1-ol (read-across): 96hr LC_{50} of >100 mg/L (Ref 23),
   b). octadecan-1-ol: measured 96hr LC_{50} of >1000 mg/L (Ref 22),
   c). docosan-1-ol (read-across): 96hr LC_{50} of >100 mg/L (Ref 23), measured 96hr LL_{50} of >1000 mg/L WAF (water accommodated fraction) (Ref 25).

   Adequate reliable measured data exists for short-term toxicity to fish to components of olefins polymer, oxidized, hydrolyzed, distillation residues (namely, icosan-1-ol and docosan-1-ol). In a conservative approach the most sensitive study result from across the two constituents has been identified and used to address the hazard endpoint for Nafol 22+. The most sensitive study result from across the two substances (namely, icosan-1-ol and docosan-1-ol) has been identified as a reliable study with octadecan-1-ol (Ref 22), with read-across applied to icosan-1-ol, which reports an LC_{50} for short term toxicity in fish of greater than the water solubility of octadecanol (0.0011 mg/L). This indicates that Nafol 22+ is not toxic at the limit of solubility. Note that for Ref 22 and Ref 25, only the robust study summary (RSS) of each study is available.

6. Long-term toxicity to fish
   Expert judgement: non-toxic at the water solubility limit for 1-eicosanol, 1-docosanol, and tetracosanol (Ref 23).

7. Short-term toxicity to aquatic invertebrates (Daphnia)
   a). icosan-1-ol (read-across): 96hr LC_{50} of >100 mg/L (Ref 23),
   b). docoosan-1-ol (read-across): 96hr LC_{50} of >100 mg/L (Ref 23).

   In a conservative approach the most sensitive study result from across the two constituents has been identified and used to address the hazard endpoint for Nafol 22+, with the 96 hr LC_{50} for docosan-1-ol being predicted as >100 mg/L (Ref 23). However, this predicted LC_{50} is greater than the limit of solubility of 0.1 mg/L. Therefore, the substance is not considered to be toxic.

8. Long-term toxicity to aquatic invertebrates
   Expert judgement: non-toxic at the water solubility limit for 1-eicosanol, 1-docosanol, and tetracosanol (Ref 23).

9. Toxicity to aquatic algae
   a). icosan-1-ol (Expert judgement): 72hr EC_{50} of >100 mg/L (Ref 23),
   b). docoosan-1-ol (Expert judgement): 72hr EC_{50} of >100 mg/L (Ref 23).

   There were no reliable measured data for short-term toxicity of docosan-1-ol to algae. Expert judgement on read-across from other taxonomic groups and the alcohols category to fill gaps

(Ref 23). The read-across took account for the measured and predicted data for different trophic levels in consistent patterns in their relative susceptibilities (Ref 23). The justifications of the read-across method for gap filling have been used in the alcohols category for Long Chain Alcohols (LCA) under REACH (Ref 21).

10. Terrestrial plant toxicity
There is no need for the terrestrial plant toxicity study as Nafol 22+ rapidly degrades in the environment. A waiver for the study was used for REACH and is well justified.

11. Effects on soil microorganisms
There is no need for the soil micro-organisms study as Nafol 22+ rapidly degrades in the environment. A waiver for the study was used for REACH and is well justified.

12. Long-term toxicity to sediment organisms
There is no need for the long-term toxicity to sediment organisms study as Nafol 22+ rapidly degrades in the environment. A waiver for the study was used for REACH and is well justified.