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 (C6-24 ALCOHOLS CATEGORY REPORT – ECOTOXICITY, 2016). 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 (Ready Biodegradability: CO_2 Evolution Test). The test substances were icosan-1-ol, docosan-1-ol, and 2-decyltetradecanol. There were 84.9% - 88.4% degradation at the end of the tests (28 days) and the test substances also achieved 60% degradation within the 10-day window in both tests. 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 estimated using the SRC PCKOCWIN method, with the K_{oc} = 43800 for 1-eicosanol and K_{oc} = 149000 for 1-docosanol.

4. Bioaccumulation in aquatic specie
   The calculated BCF = 31800 for both 1-eicosanol and 1-docosanol (Connell and Hawker, 1988).

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 (Fisk et al., 2009),
   b). octadecan-1-ol: measured 96hr LC_{50} of >1000 mg/L (Wetton, 1996),
   c). docosan-1-ol (read-across): 96hr LC_{50} of >100 mg/L (Fisk et al., 2009), measured 96hr LL_{50} of >1000 mg/L WAF (water accommodated fraction) (Wetton, 2000).

   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 (Wetton 1996), 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.

6. Long-term toxicity to fish
   Expert judgement: non-toxic at the water solubility limit for 1-eicosanol, 1-docosanol, and tetracosanol (Fisk et al. 2009).

7. Short-term toxicity to aquatic invertebrates (Daphnia)
   a). icosan-1-ol (read-across): 96hr LC_{50} of >100 mg/L (Fisk et al., 2009),
   b). docoosan-1-ol (read-across): 96hr LC_{50} of >100 mg/L (Fisk et al., 2009).

   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 (Fisk et al., 2009). 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 (Fisk et al. 2009).

9. Toxicity to aquatic algae
   a). icosan-1-ol (Expert judgement): 72hr EC_{50} of >100 mg/L (Fisk et al., 2009),
   b). docoosan-1-ol (Expert judgement): 72hr EC_{50} of >100 mg/L (Fisk et al., 2009).

   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 (Fisk et al., 2009). The read-across took account for the measured and predicted data for different trophic levels in consistent patterns in their relative susceptibilities (Fisk et al., 2009). The justifications of the read-across method for gap filling have been used in the alcohols category for Long Chain Alcohols (LCA) under REACH (C6-24 ALCOHOLS CATEGORY REPORT – ECOTOXICITY, 2016).

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 microorganisms 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.