SIDS INITIAL ASSESSMENT PROFILE

Alfa Olefin Category

CAS No.	592-41-6	111-66-0	872-05-9
Chemical Name	1-hexene	1-octene	1-decene
Structural Formula	CH_2=CH-$(CH_2)_3$-CH_3	CH_2=CH-$(CH_2)_5$-CH_3	CH_2=CH-$(CH_2)_7$-CH_3
CAS No.	112-41-4	1120-36-1	
Chemical Name	1-dodecene	1=tetradecene	
Structural Formula	CH_2=CH-$(CH_2)_9$-CH_3	CH_2=CH-$(CH_2)_{11}$-CH_3	

RECOMMENDATIONS

The chemicals are candidates for further work.

SUMMARY CONCLUSIONS OF THE SIAR

Category Definition

This profile includes an evaluation of SIDS-level testing data, using a category approach, with five individual monoolefins (1-hexene, 1-octene, 1-decene, 1-dodecene, and 1-tetradecene). For the purposes of the OECD SIDS Programme, the category was defined as olefins bearing a single medium-length (C_6 – C_{14}), even-numbered, unbranched aliphatic chain with no other functional groups.

Human Health

Based on screening level tests, all five alpha olefins have been tested and indicate low toxicity concerns for acute oral, dermal and inhalation exposure. These materials are slightly irritating to the skin and eyes of rabbits. In repeated dose studies, 1-hexene, 1-octene and 1-tetradecene have shown comparable levels of low toxicity to female rats (alterations in body and organ weights and changes in certain hematological values) at the higher doses tested (NOAELs of $\geq$ 100 mg/kg oral or $\geq$ 1000 ppm inhalation) and male rat-specific kidney damage that is likely associated with the $alpha_{2u}$-globulin protein (LOAELs $\geq$ 100 mg/kg oral only). Based on screening level testing, they appear not to be neurotoxic (for 1-hexene and 1-tetradecene), produce no adverse effects on reproduction or fetal development (1-hexene and 1-tetradecene), and are not genotoxic (all five of the alpha olefins). As a result, all the above tested endpoints indicate a low hazard potential for human health.

Environment

The potential for exposure of aquatic organisms to C_6-C_{14} alpha olefins will be influenced by their physicochemical properties. The predicted or measured water solubilities of these alpha olefins range from 50 mg/L at 20^0C for 1-hexene to 0.0004 mg/L at 25^0C for 1-tetradecene, which suggests there is a

lower potential for exposure to the higher alpha olefins due to their low solubility. Their vapor pressures range from 140 mmHg at 20^0C for 1-hexene to 0.015 mmHg at 25^0C for 1-tetradecene, which suggests the lower alpha olefins will tend to partition to the air at a significant rate and not remain in the other environmental compartments for longer periods of time.

Several acute aquatic toxicity studies show that 1-hexene and 1-octene have LC/EC50 values below their respective water solubility values (1-hexene: 96 hour LC50 in rainbow trout of 5.6 mg/L and 1-octene: 24 hour EC50 in daphnids of 3.2-10 mg/L). The daphnid value is from an experiment using less than standard exposure conditions (24 hours versus 48 hours). Chronic aquatic toxicity may occur for all of the alpha olefins except 1-tetradecene (predicted 30 day fish toxicity values range from 0.5 to 0.004 mg/L for 1-hexene and 1-dodecene, respectively. Algal toxicity studies were done with all five category members, but the most valid data were with 1-hexene (96 hour EC50 of 22 mg/L). A better understanding of whether these materials are released to water and at what quantities will determine the need to perform chronic aquatic toxicity testing.
Biodegradation data confirm that the C_6-C_{14} alpha olefins degrades in soil and water. They are also expected to degrade in the atmosphere at a rapid rate based on their atmospheric oxidation potentials. Consideration of these degradation processes supports the assessment that these substances will degrade relatively rapidly in the environment and not persist.

Exposure

C_6 – C_{14} Alpha-olefins are major industrial products, which are primarily used as intermediates in the production of the other chemicals and polymers. Other emerging uses are as components of some drilling fluids, and as potential replacements for certain hydrocarbon solvents. Occupational exposures are most likely by the inhalation and dermal routes. Inhalation exposures from industrial manufacture and commercial use are generally considered to be minimal (less than 1 ppm) under normal working conditions. The lower alkenes are minor components of gasoline, or are produced incidentally in combustion of gasoline and polymers, so their presence has been detected in urban air. Such levels were reported to be in the ppb range with a maximum reported value of 0.1 ppm. These alkenes also occur in natural products, although no quantitative values have been reported.

Non-occupational human exposure to alpha olefins is not expected since the compounds are used as industrial intermediates. Atmospheric emissions of alpha olefins from manufacturing are expected to be small and to result primarily from fugitive emission sources originating from compromised hardware (i.e.. faulty seals prior to repair) used in production and storage. On-site waste treatment processes are expected to remove these compounds from aqueous waste streams to the extent that they will not be detectable in effluent discharge. Alpha Olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes. Therefore, environmental exposure to the environment is expected to be minimal.

Category Discussion/Conclusions

A category analysis was done for all the SIDS endpoints by examining available data to determine whether the proposed test plan – to treat the five chemicals as a category – was satisfactory. Results indicate that they were and so no further SIDS-level testing is necessary.

The data indicate an increasing or decreasing trend or pattern from the shortest category member (C_6) to the longest category member (C_{14}) for various physicochemical properties and ecotoxicity (using a mixture of experimental data and estimation techniques), whereas there appears to be no difference across category members for biodegradation and health endpoints.

Melting point, vapor pressure, and water solubility decrease with increasing chain length while boiling point and octano:water partition coefficients increase with increasing chain length. Measured and predicted acute aquatic toxicity data indicate that 1-hexene, 1-octene, and 1-decene exhibit acute effects to aquatic organisms at levels at or below their water solubility; whereas 1-dodecene and 1-tetradecene

are not likely to be acutely toxic, probably because they cannot achieve a high enough water concentration to produce acute effects below their water solubility. Predictions of chronic aquatic toxicity suggest that 1-hexene may be less toxic than the rest of the category members and 1-octene, 1-decene, and 1-dodecene are expected to be similarly toxic (estimated values within approximately one order of magnitude among them). The model used (ECOSAR) could not predict the chronic aquatic toxicity of 1-tetradecene. There is no apparent difference regarding biodegradability; available data on four/five category members indicate there are no significant differences among the group. Data presented relative the health effect endpoints of the $C_6 - C_{14}$ alpha olefins indicate no differences among the five category members for acute toxicity, repeat dose toxicity, genotoxicity and reproductive/developmental toxicity.

Given the fact that not all category members were tested for each SIDS endpoint, this analysis shows that where test data exist for more than one category member, it is reasonable to interpolate (and sometimes extrapolate) for the same endpoint(s) to untested category members. Thus, it is not necessary to test each category member for all SIDS endpoints. It is concluded that using a category approach to evaluate the SIDS-level endpoints for the five alpha-olefins identified above was successful.

NATURE OF FURTHER WORK RECOMMENDED

Further work is recommended in the environmental area. There are no measured data available for chronic toxicity to aquatic organisms, however, computer modelling suggests that 1-octene,1-decene and 1-dodecene may be highly toxic (Chronic value<0.1 mg/L) under chronic exposure conditions. Therefore it is recommended that further data be collected from member countries regarding actual release data from manufacturing and processing facilities to the water compartment at local and national levels. In the event that releases to the water compartment are occurring at levels anticipated to pose a hazard to the aquatic environment, then consideration should be given to determining if chronic aquatic (including sediment-dwelling organisms) toxicity testing would be appropriate.