INTEROFFICE COMMUNICATION

TO: File for Dicyclopentadiene (CAS # 77-73-6)

FROM: Robert Sills, AQD Toxics Unit Supervisor

SUBJECT: Dicyclopentadiene ITSL change in the averaging time from 24 hrs to annual

DATE: September 14, 2015

The current ITSL for dicyclopentadiene (1 ug/m³) has a justification (attached) dated June 12, 2012. The averaging time (AT) assigned at that time was 24 hours, as per the default methodology (Rule 232(2)(b)). The current file review concludes that the AT may appropriately be set at annual, based on the nature and duration of the key study and the ITSL value derivation, as allowed under Rule 229(2)(b). Therefore, the AT is being changed from 24 hours to annual at this time.

MICHIGAN DEPARTMENT OF ENVIRONMENTAL QUALITY

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TO: File for Dicyclopentadiene (CAS# 77-73-6)

FROM: Michael Depa and Doreen Lehner, Toxics Unit, Air Quality Division

- SUBJECT: Screening Level Determination for Dicyclopentadiene
- DATE: June 12, 2012

The initial threshold screening level (ITSL) for dicyclopentadiene is 1 μ g/m³ based on a 24-hour averaging time.

Dicyclopentadiene (DCPD) [CAS#77-73-6] has a molecular formula of $C_{10}H_{12}$, is a tricyclic compound with a molecular weight of 132.2 g/mol, and is a colorless liquid or solid with a disagreeable camphor-like odor and is a side-product of the steam cracking of naptha and gas oils to produce ethylene. Dicyclopentadiene is used in aromatic hydrocarbon resins, unsaturated polyester resins, phenolic resins, epoxy resins, latexes, cyclic olefin copolymers, reaction/injection molding resins, ethylene-propylene-diene rubbers, flame retardant in plastics, an intermediate in insecticides, antioxidants, catalysts, inks, adhesives, paints, varnishes and an intermediate in flavors and fragrances (VDH, 2004; Dow, 2009). Below is the structure for dicyclopentadiene.



Figure 1. Ball and stick model of dicyclopentadiene.

A literature review was conducted to determine an initial threshold screening level (ITSL) for dicyclopentadiene. The following references and databases were searched to derive the above screening level: Chemical Criteria Database (CCD), United States Environmental Protection Agency (US EPA) Integrated Risk Information System (IRIS), National Institute for Occupational Safety and Health (NIOSH), American Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Values and Biological Exposure Indices (TLV/BEI) 2010 guide, National Toxicology Program (NTP) Study Database, International Agency for Research on Cancer (IARC) Monographs, Acute Database, Chemical Abstract Service (CAS) Online

(6/7/2012), National Library of Medicine (NLM) online, EPA Aggregated Computational Toxicology Resource (ACToR) Database, EPA Toxic Substance Control Act Test Submission Database (TSCATS), Registry for Toxic Effects of Chemical Substances (RTECS), and Health Effects Assessment Summary Tables (HEAST). The EPA has not established a reference dose (RfD) or a reference concentration (RfC) for dicyclopentadiene. Both the ACGIH TLV and the NIOSH REL are 5 ppm (27 mg/m³).

ACGIH TLV Documentation

The TLV for dicyclopentadiene has been 5 ppm (27 mg/m³) since 1976 (ACGIH, 2001). Among other data, the ACGIH TLV Documentation lists the chemical and physical properties of dicyclopentadiene. The vapor pressure of dicyclopentadiene is 1.4 torr at 20°C. The odor threshold is 0.003 ppm (16 µg/m³), but is not noticeably irritating below 5 ppm. Dicyclopentadiene is insoluble in water. ACGIH states that the acute toxicity varies greatly with the route of entry, with oral as "extremely high" (ACGIH, 2001).

Toxicological Reports

Human Studies

In a plastic manufacturing facility, men exposed to dicyclopentadiene, along with other chemicals had more female than male children. There was a significant excess of female births (6 males and 18 females, p<0.01) among the workers. There was neither congenital deformity nor disease among the offspring (Okubo et al., 2000).

As summarized by ACGIH (2001), two human subjects were exposed to 1 ppm (5.4 mg/m³). One subject experienced mild eye and throat irritation in 7 minutes and the other experienced olfactory fatigue in 24 minutes. However, ACGIH stated that no fatigue occurred in either subject during a 30-minute exposure at 5.5 ppm.

Animal Studies

In a 90 day inhalation study, groups of 51 male and female Fischer 344 rats and 45 male and female B5C3F1 mice were exposed to 0, 1, 5.1, or 51 ppm (0, 5.4, 28, or 276 mg/m³) for 13 weeks (64 exposures) for 6 hours per day, 5 days per week (Union Carbide, 1983). Sacrifices were made at 29 and 92 days post-exposure. Extensive analysis was made of urine, blood chemistry, clinical observations, organ weights, histopathology, hematology, food and water consumption and gross pathology. Approximately 20% of the mice died in the 51 ppm dose group. The primary cause of death was attributed to pulmonary congestion, although no lung lesions were found. Body weights and weight gains were comparable to controls except for female mice exhibiting body weight gains at the end of exposure, however, these gains returned to control levels by the end of the post-exposure period. Lacrimation, pariorbital hair loss, discharge or encrustations appeared in a few female rats of all three dicyclopentadiene test levels during the post-exposure recovery period and not in the control rats. Serum albumin decreased by roughly 7% in the female mice exposed to 5.1 and 51 ppm (sacrificed after 64th exposure). Absolute and relative liver weights in female mice were increased at the 5.1 ppm dose group, however, the authors stated that following histopathological examination no morphological changes were found to be associated with exposure. This held true for female rats whose relative liver weights were increased after 10, 30, and 64 exposures to 51 ppm. Female rats also had decreased activity in serum alanine aminotransferase after 64 exposures in the 5.1 and 51 ppm dose groups. The authors stated that microscopic examination again showed there were no dicyclopentadiene-related lesion differences compared to control female rats (Union carbide, 1983).

Derivation of Reference Concentration

The 13-week study in rats and mice is the best study available to estimate chronic inhalation toxicity. The dose levels of 5.1 and 51 ppm dicyclopentadiene produced adverse effects after the 64th exposure which included decreased serum albumin (p<0.05) in female mice and decreased activity in serum alanine aminotransferase (p<0.05) in the female rats. Also, in the female rats, lacrimation, pariorbital hair loss, discharge or encrustations during the post-exposure recovery at all dose levels, which were not seen in control rats. The 5.1 ppm dose was determined to be the lowest observable adverse effect level (LOAEL). The 1 ppm dose was determined to be the no observable adverse effect level (NOAEL). The RfC was then derived according to EPA RfC methodology (EPA, 1994), as follows:

The exposure dose (NOAEL_{exp}) of 1 ppm was first converted to 5.4 mg/m³. The exposure dose in mg/m³ is equal to

$$\frac{mg}{m^3} = \frac{1 \ ppm \ x \ MW}{24.45}$$

Where:

MW is the molecular weight of dicyclopentadiene in grams (MW of dicyclopentadiene is 132.2 g/mol).

$$\frac{mg}{m^3} = \frac{1\,ppm \times 132.2\,g}{24.45} = 5.4\,\frac{mg}{m^3}$$

The NOAEL_{exp} identified in the study was duration adjusted to account for continuous exposure resulting in a NOAEL _{adj}. Using the hours exposed per day and days per week.

$$\begin{split} \text{NOAEL}_{adj} &= \text{NOAEL}_{exp} \times \frac{6 \text{ hours}}{24 \text{ hours}} \times \frac{5 \text{ days}}{7 \text{ days}} \\ \text{NOAEL}_{adj} &= 5.4 \frac{mg}{m^3} \times \frac{6 \text{ hours}}{24 \text{ hours}} \times \frac{5 \text{ days}}{7 \text{ days}} \\ \text{NOAEL}_{adj} &= 0.9643 \frac{mg}{m^3} / m^3 \end{split}$$

Since dicyclopentadiene is a category 3 gas (insoluble in water, relatively unreactive), the Human Equivalent Concentration (HEC) is the same as the $NOAEL_{adj}$. The RfC is then calculated accordingly:

$$RfC = \frac{NOAEL_{HEC}}{(UF_1 \times UF_2 \times UF_3)}$$

Where:

UF1 is 10 to account for sensitive individuals, UF2 is 10 to convert from a subchronic to chronic duration, UF3 is 10 to convert the exposure dose from animal to human.

$$RfC = \frac{\frac{0.96^{mg}}{m^3}}{\frac{(10 \times 10 \times 10)}{RfC = 0.0009643^{mg}}}_{RfC = 1^{\mu g}}$$

Based on Rule 232(1)(a) the ITSL is equal to the RfC. Based on Rule 232(2)(b), the averaging time is 24-hours. Therefore, the ITSL for dicyclopentadiene is 1 μ g/m³ based on a 24-hour averaging time.

References:

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