Texas Commission on Environmental Quality Response to Public Comments

November 2013 Revised n-Butyl Acetate Development Support Document

The American Chemistry Council's Oxo Process Panel ("the Oxo Panel") submitted comments dated March 10, 2014 on the revised Development Support Document for n-butyl acetate. The Texas Commission on Environmental Quality (TCEQ) appreciates the effort put forth by the Oxo Panel to provide technical comments on the proposed DSD for n-butyl acetate. The goal of the TCEQ is to protect human health and welfare based on the most scientifically-defensible approaches possible (as documented in the DSD), and evaluation of these comments furthered that goal. A summary of comments from the Oxo Panel is provided below, followed by TCEQ responses. The full comments are provided in Appendix 1. Comments on issues that suggest changes in the DSD are addressed whereas comments agreeing with TCEQ's approach are not. TCEQ responses indicate what changes, if any, were made to the DSD in response to the comment.

Upon further review, the DSD has not been revised.

Comment No. 1:

The Revised DSD for n-butyl acetate is scientifically sound on several issues and demonstrates TCEQ's commitment to developing supportable values.

The Panel is concerned, however, about TCEQ's approach to calculating the geometric average odor threshold concentration for n butyl actetate using data derived with different methodologies and mathematical calculations. Specifically, the geometric mean calculation combines data from the traditional method of determining an "absolute" odor threshold (i.e., the average concentration that individual panelists can detect odor on 50% of the trials) with an approach that defines a "population" odor threshold as the concentration where 50% of the panelists can detect an odor. While the apparent differences may be small, combining the two types of data can be problematic since the dilution steps in an olfactory study typically occur in log cycles, magnifying the differences between the two methods. It is likely to yield confusion and/or data that is simply not interpretable.

TCEQ Response:

The TCEQ appreciates the Oxo Panel's comments. The DSD was not revised based on these comments. As described in the Ruijten et al. (2009) and van Doorn et al. (2002) reports, an individual's odor threshold is usually defined as the concentration where this likelihood is 50%. However, the inter-individual variability of odor detectability is known to be very large. The population odor threshold is the concentration at which 50% of the population can smell the odorant. In odor research, the odor detection threshold (ODT) could be described as the concentration at which 50% of population detects a sensory stimulus. According to the TCEQ 2012 guidelines, ODT is defined as the concentrations at which 50% of the volunteers

participating in an odor panel detected the odor. The TCEQ uses all reliable population ODTs (e.g., meet Level 1 or Level 2 criteria), *not* data determined by individual's odor threshold, to set an odor-based ESL for a compound. The TCEQ uses a geometric mean value for a compound with two or more reported Level 1 or Level 2 population ODTs instead of the lowest reported population ODT to set the odor-based ESL following the NAC/AEGL Committee's guidance (TCEQ 2012). Level 1 or 2 ODT are determined by modern olfactometry standards such as the Dutch and Japanese methods reported by Hoshika et al. (1993), van Doorn et al. (2002), van Harreveld et al. (2003), or Nagata (2003). NAC/AEGL indicates that because Level 1 or Level 2 population ODTs are determined by modern standards which require minimum performance criteria, a geometric mean value from the data of one or more laboratories can be used. Odor-based ESL set at a geometric mean ODT can minimize potential variation of ODTs reported from different laboratories. The geometric mean calculation is not likely to yield confusion and/or data that are simply not interpretable.

Comment No. 2

I have enclosed a list of additional references that you may wish to include in the final document.

TCEQ Response:

The TCEQ appreciates the Oxo Panel's providing these additional references. The DSD was not revised based on these comments. Most of the references that the Oxo Panel provided relate to changes of volatile compounds in fruit, which is not directly relevant for the TCEQ DSD. The two references that deal with the toxicity of n-butyl acetate (Iregren et al. 1993 and Norris et al. 1997) were included in the original DSD.

APPENDIX 1

The American Chemistry Council's Oxo Process Panel Comments

BY ELECTRONIC MAIL

March 10, 2014

Toxicology Division, MC 168
Texas Commission on Environmental Quality
P.O. Box 13087
Austin, TX 78711-3087

Re: Proposed Development Support Document for n-Butyl Acetate, CAS Registry Number 123-86-4 (November 2013)

To Whom It May Concern:

The American Chemistry Council's Oxo Process Panel[1] ("the Panel") appreciates the opportunity to provide comments on the Texas Commission on Environmental Quality (TCEQ) revised development support document (DSD) for effects screening levels (ESL) for n-butyl acetate. The Panel understands the importance of ESLs in providing TCEQ with guidance to protect human health and welfare. The Revised DSD for n-butyl acetate is scientifically sound on several issues and demonstrates TCEQ's commitment to developing supportable values.

The Panel is concerned, however, about TCEQ's approach to calculating the geometric average odor threshold concentration for n butyl actetate using data derived with different methodologies and mathematical calculations. Specifically, the geometric mean calculation combines data from the traditional method of determining an "absolute" odor threshold (*i.e.*, the average concentration that individual panelists can detect odor on 50% of the trials) with an approach that defines a "population" odor threshold as the concentration where 50% of the panelists can detect an odor. While the apparent differences may be small, combining the two types of data can be problematic since the dilution steps in an olfactory study typically occur in log cycles, magnifying the differences between the two methods. It is likely to yield confusion and/or data that is simply not interpretable.

Thank you for the opportunity to provide these comments. I have enclosed a lt of additional references that you may wish to include in the final document. If you have any

[1] The "Oxo Process" refers to an industrial synthesis process which is used to produce alcohols and related oxygenated compounds. The Panel members include BASF Corporation, Celanese Limited The Dow Chemical Company, and Eastman Chemical Company.

questions, please do not hesitate to contact me at (703) 249-6727 or srisotto@amerciancehmistry.com.

Sincerely,

Steve Risotto

Stephen P. Risotto
Senior Director

Enclosure

Reference List

Aubert C and Chanforan C. Postharvest Changes in Physicochemical Properties and Volatile Constituents of Apricot (Prunus armeniaca L.). Characterization of 28 Cultivars. *J Agricul Food Chem* 55: 3074-3082 (2007)

Aubert C and Bourger N. Investigation of Volatiles in Charentais Cantaloupe Melons (Cucumis melo Var. cantalupensis). Characteristics of Aroma Constituents in Some Cultivars. *J Agricul Food Chem* 52: 4522-4528 (2004)

Bachmann U. **V**olatile compounds in apples dependent on harvesting date and after-ripening conditions" in *ISHS Acta Horticulturae 138: Postharvest Physiology and Storage*, XXI IHC 1983, Weichmann J (Ed).

Gonzalez M *et al.* Aroma Development during Ripening of Fragaria chiloensis Fruit and Participation of an Alcohol Acyltransferase (FcAAT1) Gene. *J Agricul Food Chem* 57: 9123-9132 (2009).

Iregren A *et al.* Irritation effects from experimental exposure to n-butyl acetate. *Am J Ind Med* 24: 727-742 (1993).

Jordon MJ et al. Volatile Components in Aqueous Essence and Fresh Fruit of Cucumis melo cv. Athena (Muskmelon) by GC-MS and GC-O. *J Agricul Food Chem* 49: 5929-5933 (20010

Lavilla T et al. Relationships between Volatile Production, Fruit Quality, and Sensory Evaluation in Granny Smith Apples Stored in Different Controlled Atmosphere Treatments by Means of Multivariate Analysis. *J Agricul Food Chem* 47: 3791-3803 (1999).

Lopez ML *et al.* Influence of Different Oxygen and Carbon Dioxide Concentrations during Storage on Production of Volatile Compounds by Starking Delicious Apples. *J Agricul Food Chem* 46: 634-643 (1999).

Menager I *et al.* Changes in Physicochemical Characteristics and Volatile Constituents of Strawberry (Cv. Cigaline) during Maturation . *J Agricul Food Chem* 52: 1248-1254 (2004).

Norris JC *et al.* Acute Inhalation Toxicity Studies of n-Butyl Acetate. *Inhal Toxicity* 9, 623-646 (1997).

Vallet A and Dorn S. Changes in Volatile Emissions from Apple Trees and Associated Response of Adult Female Coding Moths over the Fruit-Growing Season *J Agricul Food Chem* 53: 4083-4090 (2005)

Villatoro C *et al.* Long-Term Storage of Pink Lady Apples Modifies Volatile-Involved Enzyme Activities: Consequences of Production of Volatile Esters. *J Agricul Food Chem* 56: 9166-9174 (2008).