

SCREENING-LEVEL HAZARD CHARACTERIZATION

Gas Oils (See Appendix)

The High Production Volume (HPV) Challenge Program¹ was conceived as a voluntary initiative aimed at developing and making publicly available screening-level health and environmental effects information on chemicals manufactured in or imported into the United States in quantities greater than one million pounds per year. In the Challenge Program, producers and importers of HPV chemicals voluntarily sponsored chemicals; sponsorship entailed the identification and initial assessment of the adequacy of existing toxicity data/information, conducting new testing if adequate data did not exist, and making both new and existing data and information available to the public. Each complete data submission contains data on 18 internationally agreed to “SIDS” (Screening Information Data Set^{1,2}) endpoints that are screening-level indicators of potential hazards (toxicity) for humans or the environment.

The Environmental Protection Agency’s Office of Pollution Prevention and Toxics (OPPT) is evaluating the data submitted in the HPV Challenge Program on approximately 1400 sponsored chemicals by developing hazard characterizations (HCs). These HCs consist of an evaluation of the quality and completeness of the data set provided in the Challenge Program submissions. They are not intended to be definitive statements regarding the possibility of unreasonable risk of injury to health or the environment.

The evaluation is performed according to established EPA guidance^{2,3} and is based primarily on hazard data provided by sponsors; however, in preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor’s responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from one year prior to the date of the HPV Challenge submission to the present: (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, IRIS, NTP, ATSDR, IARC, EXTOXNET, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. OPPT’s focus on these specific sources is based on their being of high quality, highly relevant to hazard characterization, and publicly available.

OPPT does not develop HCs for those HPV chemicals which have already been assessed internationally through the HPV program of the Organization for Economic Cooperation and Development (OECD) and for which Screening Initial Data Set (SIDS) Initial Assessment Reports (SIAR) and SIDS Initial Assessment Profiles (SIAP) are available. These documents are presented in an international forum that involves review and endorsement by governmental authorities around the world. OPPT is an active participant in these meetings and accepts these documents as reliable screening-level hazard assessments.

¹ U.S. EPA. High Production Volume (HPV) Challenge Program; <http://www.epa.gov/chemrtk/index.htm>.

² U.S. EPA. HPV Challenge Program – Information Sources; <http://www.epa.gov/chemrtk/pubs/general/guidocs.htm>.

³ U.S. EPA. Risk Assessment Guidelines; <http://cfpub.epa.gov/ncea/raf/rafguid.cfm>.

These hazard characterizations are technical documents intended to inform subsequent decisions and actions by OPPT. Accordingly, the documents are not written with the goal of informing the general public. However, they do provide a vehicle for public access to a concise assessment of the raw technical data on HPV chemicals and provide information previously not readily available to the public.

<p>Chemical Abstract Service Registry Number (CASRN)</p>	<p><u>Sponsored Streams</u> See Appendix</p>
<p>Chemical Abstract Index Name</p>	<p><u>Sponsored Streams</u> See Appendix</p>
<p>Structural Formula</p>	<p>None Provided</p>

Summary

The Gas Oil Category includes 29 CASRNs. However, the sponsor did not provide any detailed description of chemical substances in the original or revised submissions other than indicating that these mixtures are primarily comprised of saturated or aromatic hydrocarbons with carbon numbers ranging from C9 to C30. The compositions of each of the sponsored substances may vary, and therefore each substance cannot be defined by a specific composition. Any information to substantiate this claim was not included in the original or revised submissions.

When EPA first reviewed the submission in 2003, it concluded that information supplied by the Sponsor was insufficient for purposes of justifying the Category (and therefore for purposes of proceeding with a full evaluation). Information that was specifically requested, which the Agency felt would allow it to evaluate the submission, was not subsequently submitted. This included the percentages of the heteroatom-containing compounds and 3 to 7-ring polyaromatic compounds (PACs) for each substance in the category, and chemical structures and percentages of the additives used in the substances comprising the Distillate Fuel subcategory. Since submission of the Sponsor's first submission, EPA has gained additional experience in considering and preparing hazard characterizations of petroleum streams. It considers the originally requested information essential, without which the Agency cannot properly consider whether or not the submission's justification for a category is defensible. Therefore, all SIDS-level endpoints for human health and environment cannot be evaluated at this time.

EPA does not accept the use of supporting chemicals for purposes of human health or ecotoxicity data. Because each compound is identified solely by carbon range, without more detailed information about the percentage composition for each, there are no appropriate supporting chemicals that may be used to assess hazard.

Data gaps for human health and environment for all SIDS-level endpoints were identified under the HPV Challenge Program.

The Sponsor, The American Petroleum Institute Petroleum HPV Testing Group, submitted a Test Plan and Robust Summaries to EPA for Gas Oil mixtures on November 7, 2003. EPA posted the submission on the ChemRTK HPV Challenge website on December 16, 2003 (<http://www.epa.gov/oppt/chemrtk/pubs/summaries/gasoilct/c14835tc.htm>). The Sponsor submitted revised robust summaries and a Category Assessment Document to EPA on September 2, 2011, which were posted on the ChemRTK HPV Challenge website on September 8, 2011.

EPA comments on the original submission were posted to the website on May 19, 2004. Public comments were also received and posted to the website. The Sponsor submitted updated/revised documents on December 18, 2003 (corrected CASRNs) and December 16, 2005 (added CASRN), which were posted to the ChemRTK website on March 3, 2004 and January 12, 2006, respectively. The mixtures proposed by the Sponsor as comprising a "Gas Oils category" consist of 29 CASRNs.

The Sponsor's November 7, 2003 submission proposed grouping the gas oils mixtures (all of which are complex and have variable compositions) into a category ("Gas Oils Category) and subdividing the gas oils into 1) Gas Oil Streams and 2) Distillate Fuel. The Sponsor also proposed to subdivide Gas Oil Streams into *Predominantly Saturated Hydrocarbons* and *Predominantly Aromatic Hydrocarbons*, although it did not specify which mixtures belonged to Predominantly Saturated Hydrocarbons, and which to Predominantly Aromatic Hydrocarbons.

The Sponsor's comments posted on the ChemRTK website on January 12, 2006 stated that the submission was made solely to include CASRN 64742-72-9 in the Test Plan, and that no other changes had been made to the corresponding Robust Summary. The Sponsor also stated that it was gathering more information on the Category substances and that it intended to submit a response letter and revised Test Plan and Robust Summary in 2006, which would address EPA's the Public's comments.

The Sponsor's revised robust summaries and Category Assessment Document, which were included in its September 2, 2011 submission, did not include sufficient information to inform EPA's hazard evaluation for the Gas Oil Category.

Category Justification

The Gas Oil Category includes 29 CASRNs. However, the sponsor did not provide any detailed description of chemical substances in the original or revised submissions other than indicating that these mixtures are primarily comprised of saturated or aromatic hydrocarbons with carbon numbers ranging from C9 to C30. The compositions of the sponsored substances may vary, and therefore, each substance cannot be defined by a specific composition.

The Sponsor indicated that the substances included in the submission are all similar because of similar process histories and physicochemical properties, are complex petroleum mixtures that boil between 300 and 880 °F, and are composed primarily of saturated and/or aromatic hydrocarbons with carbon numbers ranging from C9 to C30. The grouping also appears to have

been based on the Sponsor's premise that mixtures with high polycyclic aromatic compounds (PACs) content, specifically 3-7 ring PACs, correlate with developmental toxicity, mutagenicity, and carcinogenicity (and possibly reproductive toxicity).

The mixtures comprising this submission contain straight and branched chain alkanes (paraffins), cycloalkanes (naphthenes), aromatic hydrocarbons and mixed aromatic cycloalkanes, as well as additives (corrosion inhibitors, defoamers, dyes/markers, antioxidants, stability improvers, cetane improvers, detergents and anti-static additives). The Sponsor considers them to be a continuum bounded by mixtures that are composed either of predominantly saturated hydrocarbons or predominantly aromatic hydrocarbons. However, information supporting this or the toxicological basis for the grouping was not provided.

Using data from ~ 15 samples (representing ~ 5 mixtures) of the submission's 29 mixtures (<<50% of the total number of mixtures), the Sponsor found that olefins, saturates, and aromatics ranged from 0-19%, 18-86%, and 14-82%, respectively. These ranges of olefins, saturates and aromatics also include ~25 mixtures that were *not* included in this submission. No information was provided on which of the proposed subcategory or groups the 5 or so mixtures represented, and no additional compositional information was provided as to moieties included in the olefins, saturates and aromatics percentages and/or information on additives. Besides lacking information on composition, the submission did not provide adequate detail on the part of the refinery process from which the submission's mixtures originate. For example, in the submission's text, CASRN 64741-44-2 is labeled as *straight run middle distillates (petroleum)*, which the Sponsor assigned to its "Predominantly Saturated Gas Oils" Group (Group 2). The API TSCA definition of this CASRN states that it is light gas oil, which consists of a complex combination of hydrocarbons, with carbon numbers predominantly in the range of C11 - C20. While the submission reports its boiling range, it does not note whether this range occurs at atmospheric or reduced pressure. From statements made by the Sponsor in the test plan, EPA could assume both that this product results from atmospheric distillation and that this assumption holds for the entire industry. To be consistent, that approach would need to be applied to the 6 other CASRNs in this group. This would force the Agency into guessing the identity of the parent streams and whether or not the additional processing is likely to leave them with chemical compositions similar enough to justify this grouping and ultimately to justify the use of read-across to determine the toxicity endpoints for this group. Overall, the current information provided for the remaining CASRNs in this example, and many of the other CASRNs in the submission, is not sufficient for purposes of determining from which processing streams these products are derived. Therefore it is unclear what the chemical constituents are likely to be for the CASRNs of this group, as well as other subcategories and groups in this submission.

When EPA first reviewed the submission in 2003, it concluded that information supplied by the Sponsor was insufficient for purposes of justifying the category (and therefore for purposes of proceeding with a full evaluation). Information that was specifically requested, which the Agency believed would allow it to evaluate the submission, was not subsequently submitted. This included the percentages of the heteroatom-containing compounds and 3 to 7-ring polyaromatic compounds (PACs) for each substance in the category, and chemical structures and percentages of the additives used in the substances comprising the Distillate Fuel subcategory. Since submission of the Sponsor's first submission, EPA has gained additional experience in

considering and preparing hazard characterizations of petroleum streams. It considers the originally requested information essential, without which the Agency cannot properly consider whether or not the submission's justification for a category is defensible.

Justification for Supporting Chemicals

EPA does not accept the use of supporting chemicals to provide human health or ecotoxicity data. Because each substance is identified solely by carbon range, without more detailed information about the percentage composition for each, there are no appropriate supporting chemicals that may be used to assess hazard.

Appendix

Subcategories in the Gas Oils Category		
29 Category Members		
	CASRN	Chemical Abstract Index Name
Subcategory I: Distillate Fuels		
<i>Sponsored Substances (4 members)</i>		
Diesel oil	68334-30-5	None available
Fuel oil no. 2	68476-30-2	None available
Fuel oil no. 4	68476-31-3	None available
Diesel fuel no. 2 (Fuel oil no. 2-D)	68476-34-6	None available
<i>Supporting Substances (4 members)</i>		
API 79-6	No CASRN	None available
LF-7765 RI	No CASRN	None available
No. 2-DA	No CASRN	None available
No. 2 Home heating oil	No CASRN	None available
Subcategory II: Gas Oils (“Refinery Streams”)		
Group 1: Predominantly Aromatic Gas Oils		
<i>Sponsored Substances (4 members)</i>		
Light catalytic cracked distillates (petroleum)	64741-59-9 Mobil LCO API 83-07	None available.
Intermediate catalytic cracked distillates (petroleum)	64741-60-2	None available
Hydrodesulfurized light catalytic cracked distillates (petroleum)	68333-25-5	None available
Aromatic hydrocarbons, C9–17	68333-88-0	None available
Group 2: Predominantly Saturated Gas Oils		
<i>Sponsored Substances (7 members)</i>		
Straight-run middle distillates (petroleum)	64741-44-2	None available
Light hydrocracked distillates (petroleum)	64741-77-1	None available
Light thermal cracked distillates (petroleum)	64741-82-8	None available
Solvent refined gas oils (petroleum)	64741-90-8	None available
Solvent refined middle distillates (petroleum)	64741-91-9	None available
Hydrotreated middle distillates (petroleum)	64742-46-7	None available

Hydrodesulfurized middle distillates (petroleum)	64742-80-9	None available
<i>Supporting Substances (2 members)</i>		
ARCO F-188	No CASRN	None available
ARCO F-215	No CASRN	None available
Group 3: Uncategorized Gas Oils		
<i>Sponsored Substances (14 members)</i>		
Straight-run gas oils (petroleum)	64741-43-1	None available
Vacuum tower condensates (petroleum)	64741-49-7	None available
Light vacuum gas oils (petroleum)	64741-58-8	None available
Sweetened middle distillates (petroleum)	64741-86-2	None available
Chemically neutralized gas oils (petroleum)	64742-29-6	None available
Chemically neutralized middle distillates (petroleum)	64742-30-9	None available
Clay-treated distillates (petroleum)	64742-38-7	None available
Distillates, petroleum, catalytic dewaxed, middle	64742-72-9	None available
Hydrodesulfurized gas oils (petroleum)	64742-79-6	None available
Hydrodesulfurized light vacuum gas oils (petroleum)	64742-87-6	None available
Catalytic, reformer fractionator residue, low-boiling distillates (petroleum)	68477-31-6	None available
Full-range straight-run middle distillates (petroleum)	68814-87-9	None available
Heavy straight-run distillates (petroleum)	68915-96-8	None available
Straight-run, high-boiling gas oils (petroleum)	68915-97-9	None available