FACT SHEET #1: Development of Organic Emission Estimates For California's Emission Inventory and Air Quality Models

- The California Air Resources Board's (ARB's) emission inventory and photochemical air quality models both quantify organic compounds as Total Organic Gases (TOG), as well as breaking TOG down according to the organic compounds in it.

- **Total Organic Gases (TOG)** means "compounds of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate."

    - TOG includes all organic gas compounds emitted to the atmosphere, including the low reactivity, or "exempt VOC", compounds (e.g., methane, ethane, various chlorinated fluorocarbons, acetone, perchloroethylene, volatile methyl siloxanes, etc.).

    - TOG also includes low volatility or "low vapor pressure" (LVP) organic compounds (e.g., some petroleum distillate mixtures). TOG includes all organic compounds that can become airborne (through evaporation, sublimation, as aerosols, etc.), excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate.

- Total Organic Gas emissions are reported in the ARB's emission inventory and are the basis for deriving the Reactive Organic Gas (ROG) emission estimates, which are also reported in the inventory.

    - ROG means TOG minus ARB's "exempt" compounds (e.g., methane, ethane, CFCs, etc.).

    - ROG is similar, but not identical, to U.S. EPA's term "VOC", which is based on EPA's exempt list. Also, various regulatory uses of the term "VOC", such as that for consumer products, exclude specific, additional compounds from particular control requirements.

- Speciation profiles are used to estimate the amounts of various organic compounds that make up TOG. A speciation profile contains a list of organic compounds and the weight fraction that each compound composes of the TOG emissions from a particular source type. Each process or product category is keyed to one of several hundred currently available speciation profiles. The speciation profiles are applied to TOG to develop both the photochemical model inputs and the emission inventory for ROG.

    - To the extent possible given available data, ARB's organic gas speciation profiles contain all emitted organic species that can be identified (ideally, detected to very low levels). This includes reactive compounds, unreactive and "exempt" compounds, and to the extent the data are available, "low vapor pressure" compounds. Research studies are conducted regularly to improve ARB's species profiles. These profiles support ozone modeling studies but are also designed to be used for aerosol modeling. The profiles are also used to support other health or welfare related modeling studies where the compounds of interest cannot always be anticipated. Therefore, organic gas emission profiles should be as complete and accurate as possible.

- The speciation profiles used in the emission inventory are available from the ARB's web site at www.arb.ca.gov. ARB has an ongoing effort to update speciation profiles as data become available, such as through testing of emission sources or surveys of product formulation. New speciation data generally undergo technical and peer review, and updating of the profiles is coordinated with users of the data.

Prepared by the California Air Resources Board, Planning and Technical Support Division, Modeling and Meteorology Branch and Emission Inventory Branch, August 2000.

FACT SHEET #2: Handling of Organic Compounds in California's Photochemical Air Quality Modeling

- The California Air Resources Board's (ARB's) photochemical air quality models and ARB's emission inventory both quantify organic compounds as Total Organic Gases (TOG).

- Photochemical models simulate the processes leading to ozone formation and fate in the lower atmosphere, and, to be realistic, must include all compounds emitted to the atmosphere. Therefore, ARB's modeling procedures require Total Organic Gas emissions as the input.

- ARB's chemical speciation profiles[1] are applied to characterize the chemical composition of the total organics emitted from each source type.

- For State Implementation Plan (SIP) attainment demonstrations and evaluations, the California Air Resources Board's photochemical air quality models have been approved by the U.S. EPA. The photochemical air quality models used by the ARB for SIP attainment demonstrations use the Carbon Bond IV photochemistry[2] and/or other chemical mechanisms.

- Both U.S. EPA's and ARB's models use total organic gases, which include the "exempt VOCs", and, to the extent data have been available, any low vapor pressure compounds that become airborne.

- The photochemical models contain lumped chemical mechanisms which assign appropriate reactions and reaction rate constants to all compounds in the speciation profiles. These mechanisms are based on extensive scientific research and are documented in the scientific literature.

- Model results for ozone non-attainment areas have demonstrated that even compounds with low photochemical reactivity or low vapor pressure contribute to photochemical ozone formation.

    - For example, even an "exempt VOC" like ethane has been shown to have a contribution to ozone formation. If all exempt compounds and low vapor pressure compounds were omitted from photochemical model simulations, the ozone attainment demonstration would be compromised.

    - The model takes into account that, individually, compounds with low reactivity or that are present in small amounts have a small impact on ozone formation. However, the cumulative effect of several low reactive compounds or many low emission compounds can be a significant contribution to photochemical ozone formation.

REFERENCES:

1. ARB Speciation Profiles: (a) California Air Resources Board, "Identification of Volatile Organic Compound Species Profiles: ARB Speciation Manual, Second Edition, Volume 1 of 2," August 1991; and (b) subsequent revisions. The latest ARB speciation profiles are available from ARB's web site at www.arb.ca.gov.

2. Carbon Bond IV: Morris, R.E. and Meyers, T. E., "User's Guide for the Urban Airshed Model," Volume I, Appendix 1: "The Carbon Bond IV Chemical Kinetics Mechanism for Urban and Regional Scale Computer Modeling," EPA-450/4-90-007A, June 1990.

Prepared by the California Air Resources Board, Planning and Technical Support Division, Modeling and Meteorology Branch and Emission Inventory Branch, August 2000.