Introduction
Sources of organic compounds, such as wood burning, gasoline exhaust, and diesel combustion can emit gas-phase intermediate volatility compounds (IVOCs, saturation concentrations ~10^6 µg/m³). These compounds include species such as long-chain alkanes (~C12-C19 n-alkanes) as well as polycyclic aromatic hydrocarbons (PAHs, e.g. naphthalene). After emission to the atmosphere, these compounds can oxidize to form lower volatility species (~10^5 µg/m³). These compounds include species such as long-chain alkanes (indicative of IVOC volatility) from Schauer et al. [1999, 2001, 2002].

After emission to the atmosphere, these compounds can oxidize to form lower volatility compounds that partition to the aerosol phase. The yield of aerosol from these compounds depends on their structure as well as the conditions under which they are oxidized (high-NOx compounds that partition to the aerosol phase. The yield of aerosol from these compounds depends on their structure as well as the conditions under which they are oxidized (high-NOx vs low-NOx).

Current CMAQ treatment of intermediate volatility compounds: CMAQ v4.7.1 treats SOA from alkanes (including intermediate volatility alkanes) in the SAPRC mechanism. Although not explicitly treated, many PAHs are contained within existing emissions that have SOA yields based on xylene.

Objectives:
• Update the parameterization for SOA from alkanes to include information on the length and structure of the alkanes and add SOA from PAHs with yields according to a PAH surrogate (naphthalene).
• Estimate the contribution of alkanes and PAHs to ambient organic aerosol.

Baseline SOA Yields
Two species form the basis for the alkane and PAH SOA yields: n-dodecane (C12H26) for alkanes and naphthalene (C10H8) for PAHs. The yield of aerosol from these compounds depends on their structure as well as the conditions under which they are oxidized (high-NOx vs low-NOx).

Adjustment for Alkane Structure
Since not all alkanes behave like n-dodecane, the dodecane yield/precursor emissions are adjusted to account for different length and structure (cyclic, linear, branched) alkanes.

Emissions
SAPRC07 Species Annual Domain Wide Emissions Fraction Forming SOA
[kton/yr] [% by mass]
ALK4 2470 11%
ALK5 1860 67%
ALK2 738 10% as PAH, 90% as xylene

Surface Level Organic Aerosol
January 11-24, 2006

Summary
• Cyclic alkanes (C6 to C19) are predicted to contribute about half of the alkane SOA due to their high yields.
• IVOC alkanes (C12 to C19) contribute about 25% of alkane SOA, but could contribute more if emissions were missing from the inventory.
• Alkanes and PAHs contribute modest amounts of aerosol; together they are predicted to constitute ~10 to 20% of SOA from anthropogenic hydrocarbons during January 11-24, 2006. These parameterizations are expected to be part of CMAQv5.0.1.

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Updated CMAQ SOA Scheme
Based on Carlton et al. [2010] schematic of CMAQ v4.7.1 with updates shown in red.