



South Coast
AQMD

Volatility of Organic Compounds: Contribution to Ozone and PM_{2.5}

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Outline

- Volatility of Organic Compounds
- Measurements and Predictions of Vapor Pressure for Relevant Compounds
- Fate of Organic Compounds in the Atmosphere
 - Considerations for ozone production
 - Considerations for PM_{2.5} production



Organic Compounds in the Atmosphere

- Organics are molecules containing carbon
- May exist in the liquid phase, gas phase, and/or particle phase depending on volatility
- Typically classified by volatility

Less likely to
be found in
the particle-
phase

Decreasing Volatility
Slower Evaporation →

More likely to
be found in
the particle-
phase



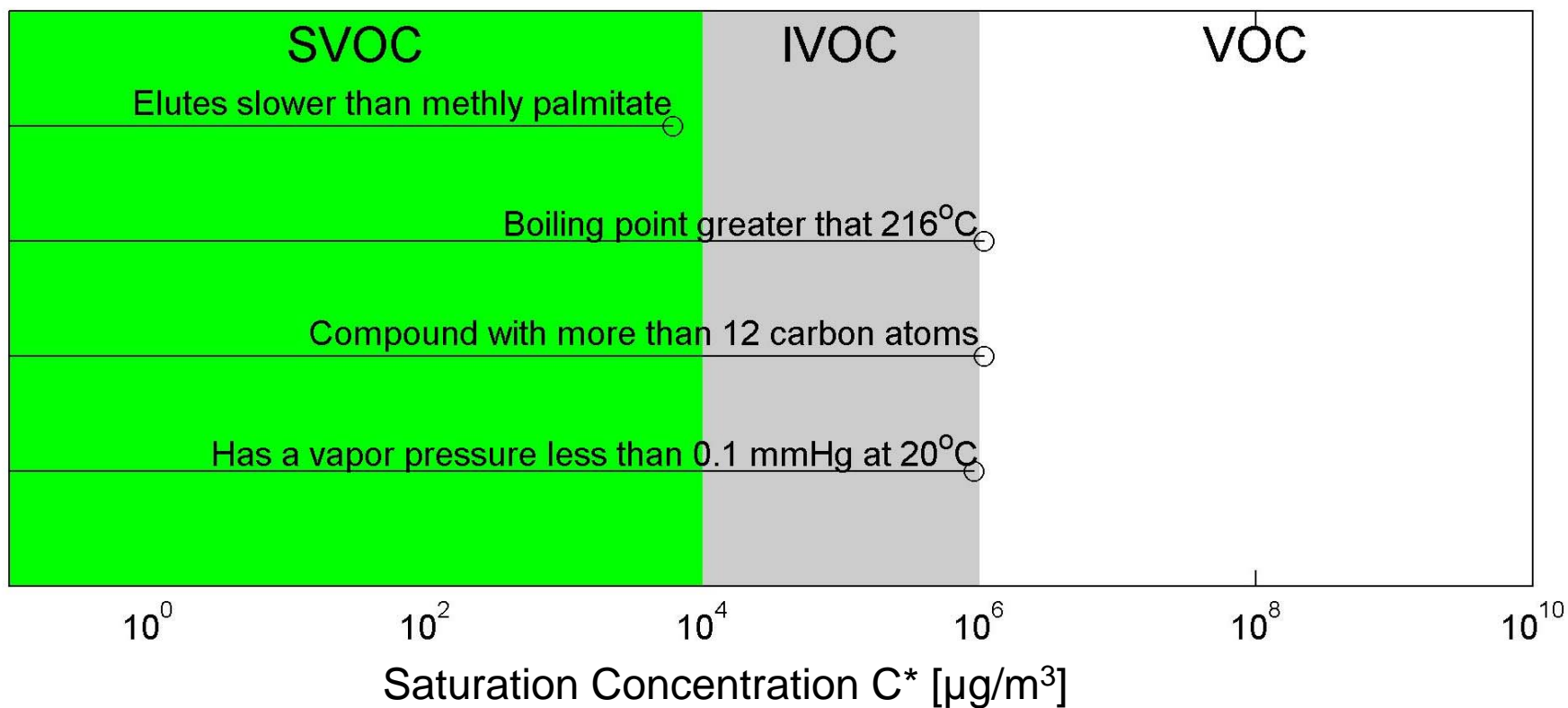
Quantification of Volatility

- Vapor Pressure, P^{VAP} [Pa]
 - Measure of the escaping tendency of a liquid
 - High vapor pressure indicates high volatility
- Saturation Concentration (C^*) [$\mu\text{g}/\text{m}^3$]
 - Vapor pressure in mass concentration units

$$C^* = \frac{P^{VAP} \cdot M_w}{R_{gas} \cdot T}$$



LVP-VOC Criteria Comparison

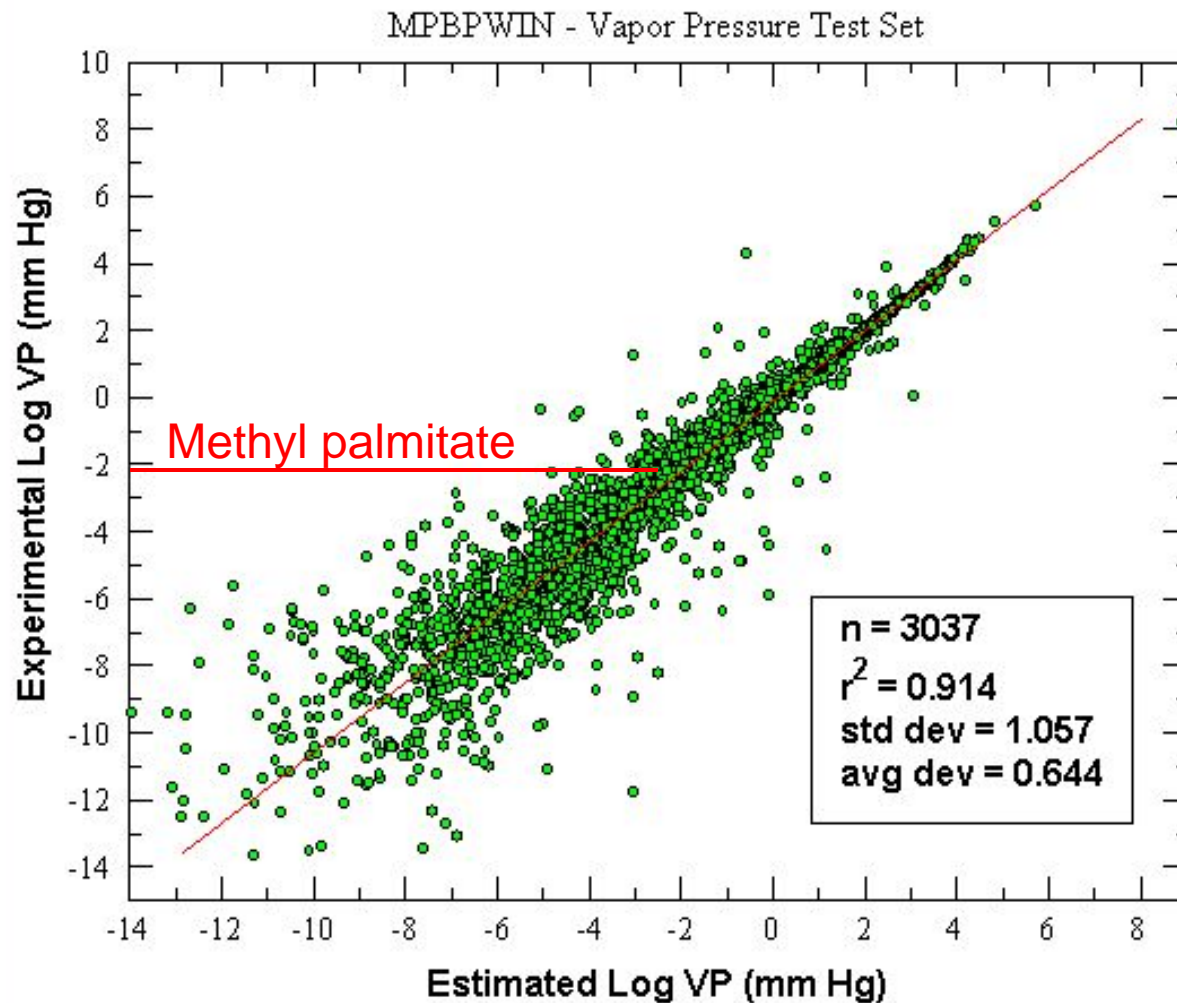


Measurements and Predictions of Vapor Pressure

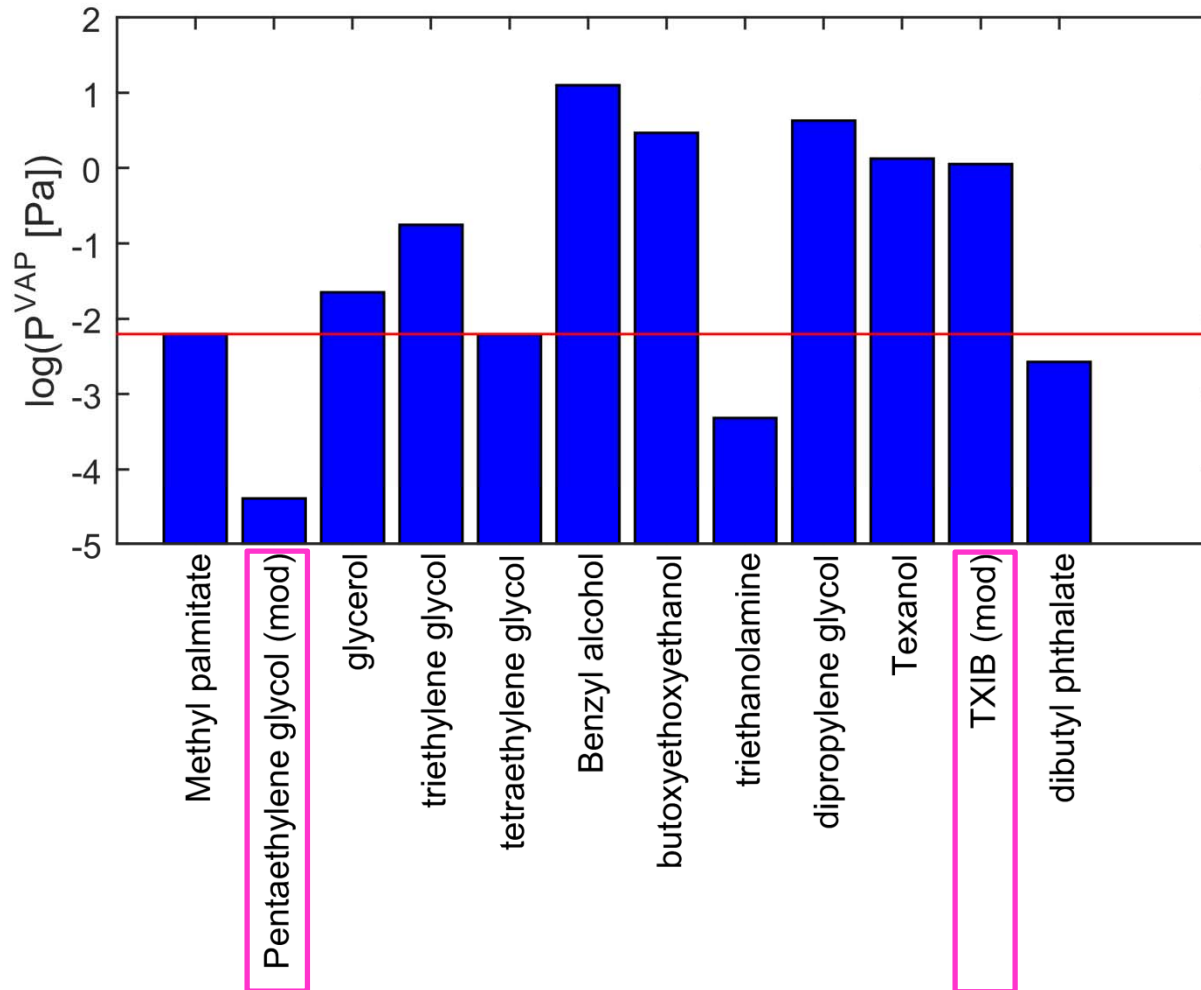
- Vapor pressures routinely measured in the laboratory
 - Measurement of IVOCs and SVOCs can be difficult
- Many techniques are available to predict vapor pressure from chemical structure and/or boiling points
 - The MPBPVP module in EPI Suite from US EPA is used to estimate vapor pressures of compounds without published values



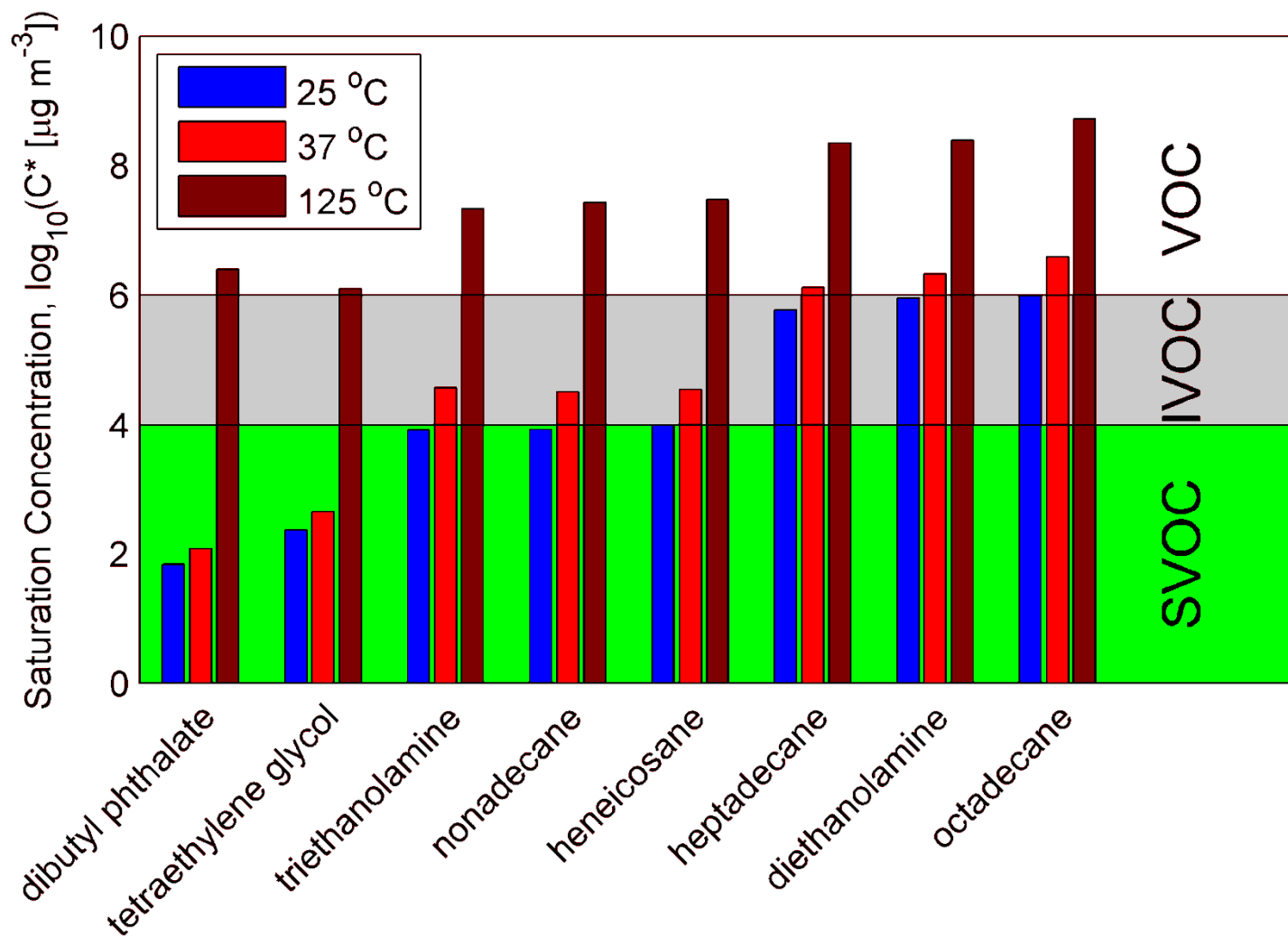
Estimation Accuracy of MPBPVP



Vapor Pressures of Relevant Compounds



Volatility is Temperature Dependent

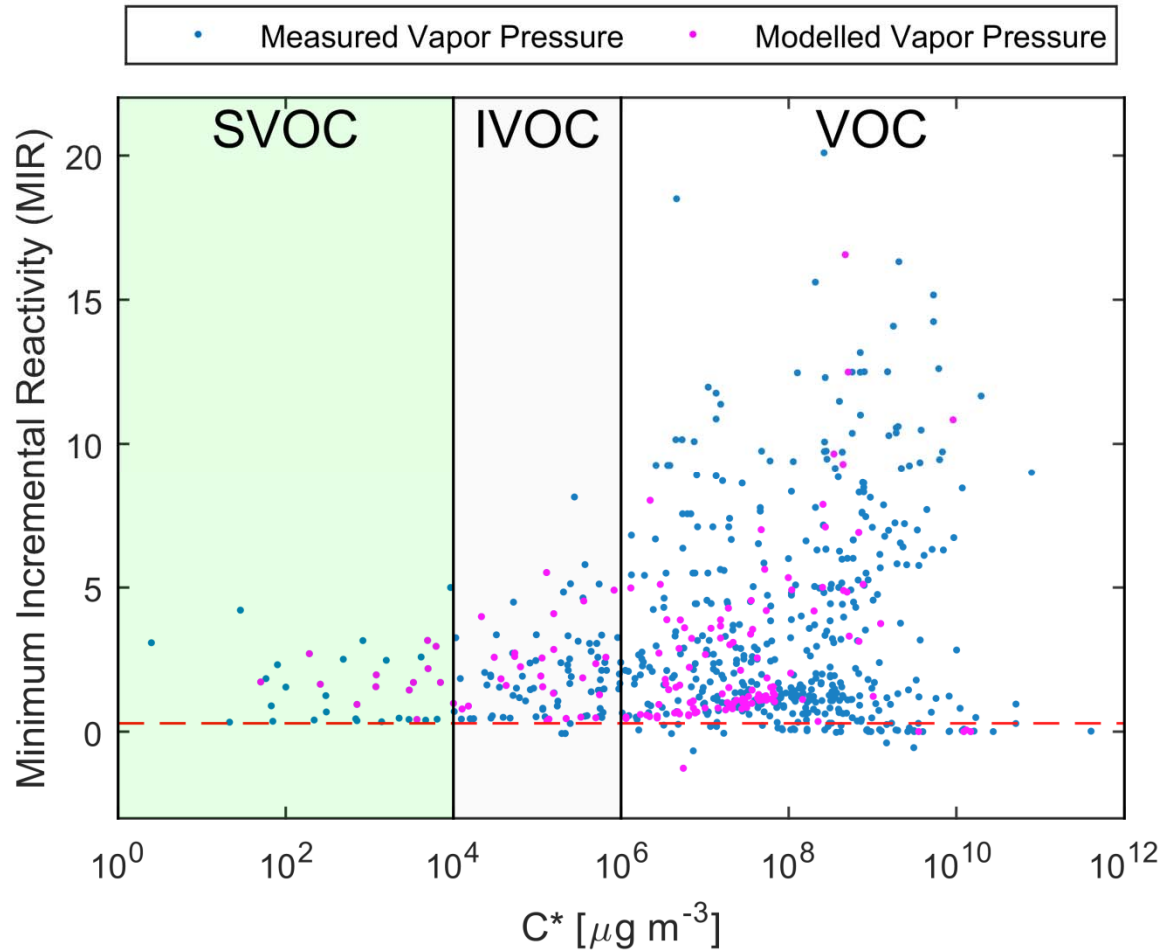


Reactivity of Organic Compounds

- Ozone Formation
 - Species dependent
 - Complex function of NO_x and VOC concentrations, sunlight intensity, and temperature
 - VOCs, IVOCs, and SVOCs can produce Ozone

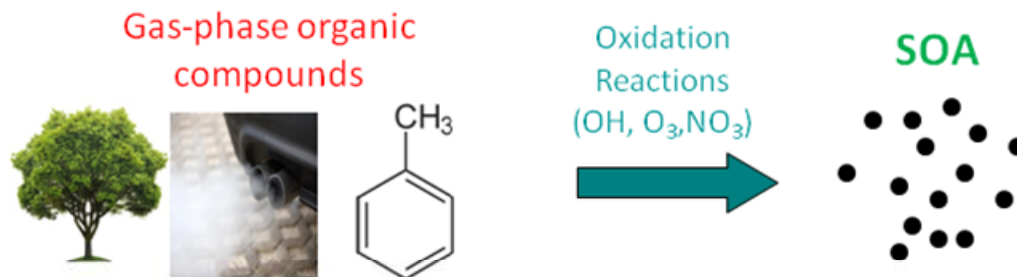


Ozone Reactivity is Not a Strong Function of Volatility

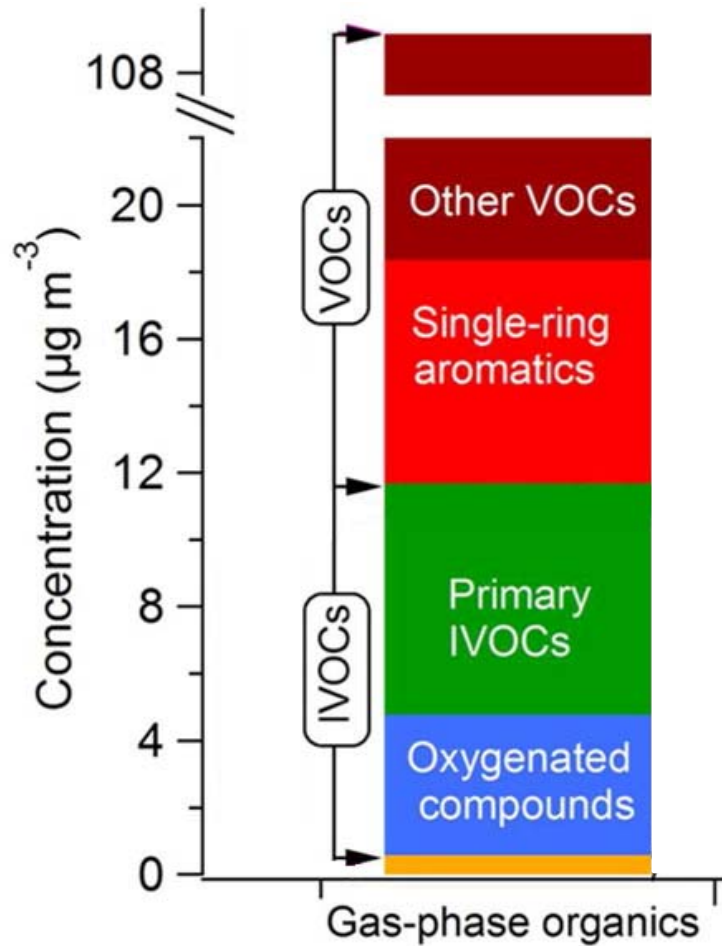


Reactivity of Organic Compounds

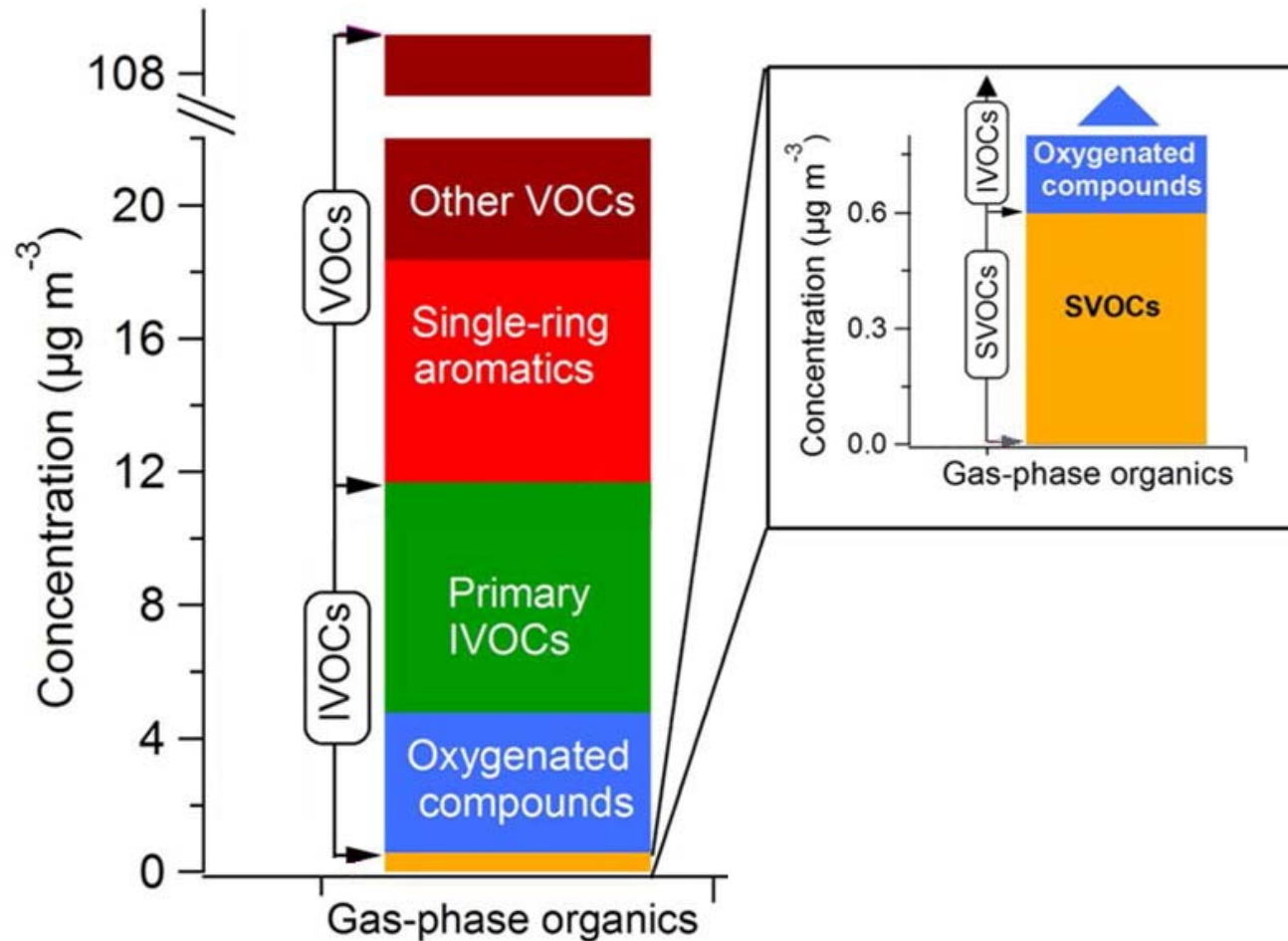
- PM_{2.5} Formation
 - Species dependent
 - VOCs, IVOCs, and SVOCs can produce PM_{2.5}
 - Primary Organic Aerosol (POA) is formed at source of emissions
 - Secondary Organic Aerosol (SOA) is formed from the oxidation of organic gases in the atmosphere



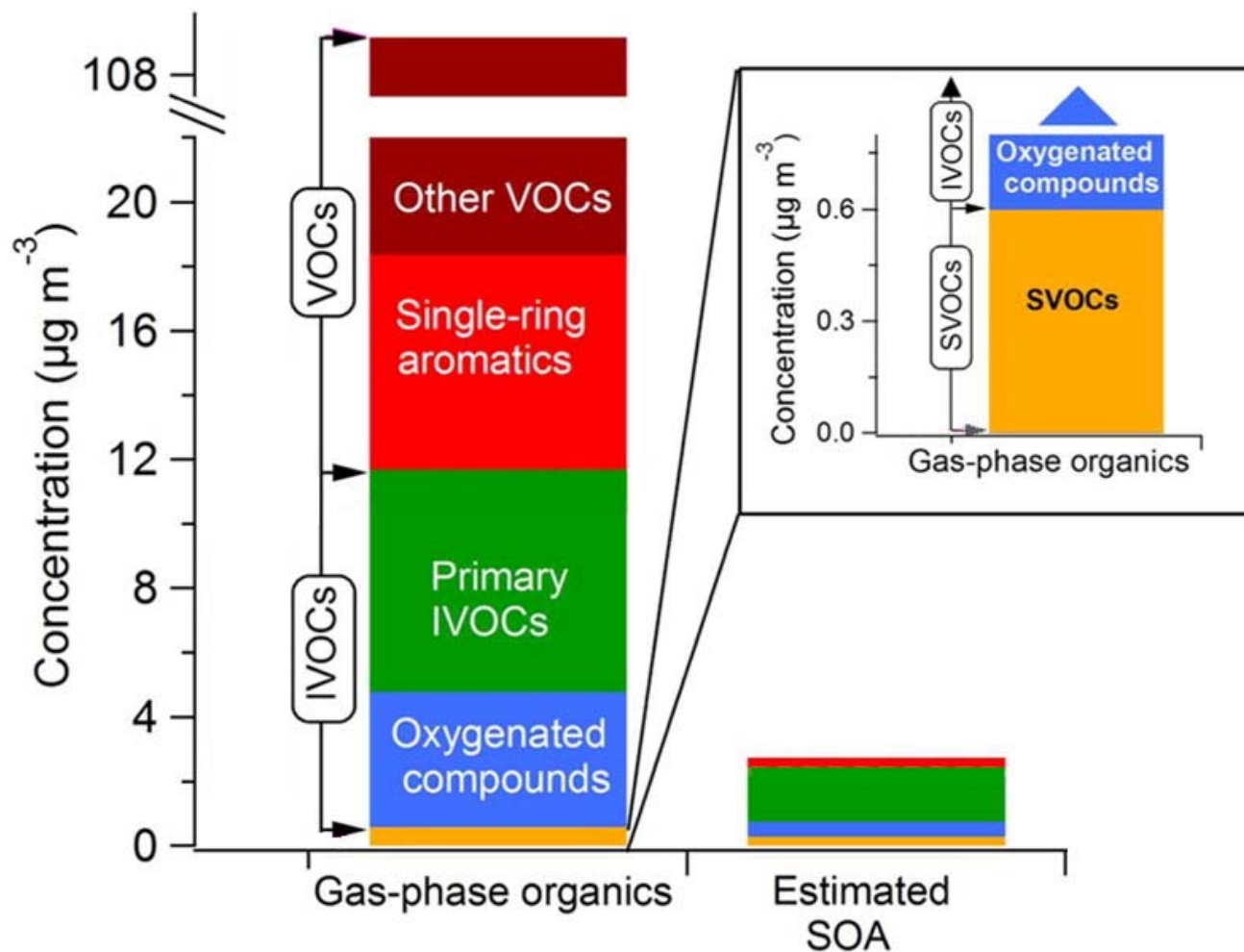
IVOC and SVOC Concentrations in Pasadena



IVOC and SVOC Concentrations in Pasadena



IVOCs and SVOCs Responsible for Majority of Ambient SOA in SoCAB



Conclusions

- Volatility of organic compounds can be measured and predicted
- IVOC and SVOC emissions inventory needed for ozone and PM_{2.5} modeling
 - Requires species-dependent and temperature-dependent evaporation rates
 - Should account for mixing effects in complex mixtures
 - Will improve accuracy of regional air quality modeling
- An accurate inventory will require more measurements of VOC, IVOC, SVOC emissions and ambient concentrations

