



## Estimates of Total Molecular Polarity to Evaluate Atmospheric Evolution of Organic Aerosol

Judith Perlinger, Paul Doskey, Rosa Flores-Rangel, Bo Zhang, and Keenan Murray  
Michigan Technological University, Houghton, United States (jperl@mtu.edu / +1 (906) 487-2943)

The relationship between the molecular composition of organic aerosol (OA) and aerosol optical properties and activation of cloud condensation nuclei (CCN), which affect the direct and indirect forcing of Earth's climate, is poorly understood. Improving our understanding of the complex relationship requires development of model parameterizations that provide adequately detailed representations of the formation and diagenesis of OA and the evolution of OA properties that affect interactions with atmospheric water. The evolution of OA depends on the molecular composition of the gas-phase solutes and the sorbing matrix of aerosols. Gas-particle partitioning can be described by five types of intermolecular interactions that solute molecules undergo with OA: size-related interactions, polar interactions, interactions resulting from excess polarizability, hydrogen bond donor, and hydrogen bond acceptor interactions, all of which are altered as OA is transformed by a series of oxidations during the atmospheric lifetime of the aerosol. Interactions of OA chemical species with water, which affect aerosol optical properties, CCN activation, and removal by precipitation, are expected to increase as the polarity/polarizability and hydrogen bond donor-acceptor (HDA) character of OA increases. However, HDA interactions with water are likely greater than interactions related to the polarity/polarizability of OA, and CCN activation is expected to increase with increasing HDA character. Pankow and Barsanti (2009; *Atmos. Environ.*, 43, 2829-2835) proposed a 2-D representation of OA chemical species to model OA formation and diagenesis that uses carbon number and total molecular polarity (tmp) as dimensions. This approach is superior to 2-D approaches that employ a 2-D space comprised of volatility and mean carbon oxidation state because the volatility of species with the same mean carbon oxidation state can vary by several orders of magnitude. The objective of the work presented here is to derive a measure of tmp from gas chromatographic retention indices of hydrocarbons with various functionalities (e.g., -OH, -CHO, C=O, -COOH, -ONO<sub>2</sub>). A comprehensive two-dimensional gas chromatographic (GC × 2GC) approach is used to determine retention indices of the organic solutes on a primary and two secondary GC columns that have stationary phases of different polarity and HDA character used as model phases for OA. Carbon number is a proxy for solute molecular size quantified using retention indices from primary column elution. Retention indices from solute elution in the two secondary columns are used to quantify molecular polarity/excess polarizability and HDA character. Polyparameter relationships for gas-particle partitioning derived from retention indices are compared with those derived from a solvation parameter model and other approaches.