



## Review

## Partitioning of volatile organic compounds to aerosols: A review

Guiying Rao, Eric P. Vejerano\*

Center for Environmental Nanoscience and Risk, Department of Environmental Health Sciences, University of South Carolina, Columbia, 29208, United States



## HIGHLIGHTS

- Partitioning of VOCs to atmospheric aerosols was reviewed.
- Nonpolar VOCs partition to the organic phase of aerosols that is insensitive to RH.
- Ionic VOCs dissolve in RH-sensitive aqueous phase of aerosols.
- Most polar VOCs partition to both organic and aqueous phases of aerosols.
- Models for estimating gas-to-particle partitioning coefficient were discussed.

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## ABSTRACT

Although volatile organic compounds (VOCs) exist mainly in the gas-phase rather than in aerosols, the concentrations of VOCs measured from aerosols are comparable to those of semi-volatile organic compounds, which preferentially partition into aerosols. VOCs that partition into aerosols may raise health effects that are generally not exerted by aerosols or by VOCs alone. So far, only scant reports on VOC/aerosol partitioning are available in the extant literature. In this review, we discuss findings presented in recent studies on the partition mechanism, factors affecting the partition process, existing knowledge gaps, and recommendations to help address these gaps for future research. Also, we have surveyed the different models that can be applied to predict partition coefficients and the inherent advantage and shortcoming of the assumptions in these models. A better understanding of the partition mechanism and partition coefficient of VOCs into aerosols can improve prediction of the global fate and transport of VOCs in the environment and enhance assessment of the health effects from exposure to VOCs.

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\* Corresponding author. 921 Assembly St., PHRC 501D, Columbia, SC, 29208 United States.

E-mail address: [vejerano@mailbox.sc.edu](mailto:vejerano@mailbox.sc.edu) (E.P. Vejerano).

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## 1. Introduction

Atmospheric aerosols are particulate matter (PM) suspended in air. Primary aerosols originate from a variety of natural and anthropogenic sources such as biomass burning, incomplete combustion of fossil fuels, volcanic eruptions, sea spray, wind-driven or traffic-related suspension of soil, mineral dust, and biological materials (plant fragments, microorganisms, pollen, etc.) (Cetin et al., 2003; Pöschl, 2005). Aerosols are transported locally, regionally or globally (Hara et al., 2010; Velasco and Rastan, 2015) with significant environmental impact on visibility (Afroz et al., 2003; Ma et al., 2012), climate (Anderson et al., 2012), and human health (Kristensen, 1989; Pope et al., 2004; Sun et al., 2010; Harrison et al., 2017). Compared to PM<sub>10</sub> (particles with aerodynamic diameter <10 μm), inhaled fine aerosol particles PM<sub>2.5</sub> (particles with aerodynamic diameter <2.5 μm) penetrate deeper into the respiratory tract (Wang et al., 2002; Nel, 2005; Valavanidis et al., 2008; Kim et al., 2015). Additionally, organic compounds partition preferentially into PM<sub>2.5</sub> compared to PM<sub>10</sub> and other larger aerosol particles (Odabasi et al., 2005). During haze episodes, the PM<sub>2.5</sub> mass concentration frequently exceeds the 24-h average National Ambient Air Quality Standard (NAAQS; [www.cpcb.nic.in](http://www.cpcb.nic.in)) and the United States Environmental Protection Agency standard of 35 μg/m<sup>3</sup> (USEPA; [www.epa.gov/air/particlepollution/](http://www.epa.gov/air/particlepollution/)). In Beijing, China (Tao et al., 2016) and New Delhi, India (Tyagi et al., 2017), the mean PM<sub>2.5</sub> during the winter of 2014 were 167 and 137 μg/m<sup>3</sup>, respectively, which are ~4 × and ~3 × higher than the NAAQS. Epidemiological studies have implicated inhaled ambient PM to a variety of respiratory and cardiovascular dysfunctions and an increase in morbidity and mortality in humans (Pope et al., 2004; Polichetti et al., 2009; Sun et al., 2010; Shrey et al., 2011; Harrison et al., 2017).

The composition and toxicity of aerosols may be altered by the partitioning of atmospheric pollutants such as VOCs (Ebersviller et al., 2012a, 2012b). A recent study reported that the use of VOCs - including pesticides, coatings, printing inks, adhesives, cleaning agents, and personal care products - constitute half of the fossil fuel VOC emissions in industrialized cities (McDonald et al., 2018). Here, we refer to VOCs as chemicals with boiling point <240 °C at a standard atmospheric pressure to differentiate them from semi-volatile organic compounds (SVOCs) that exhibit boiling point >240 °C and up to 400 °C (US EPA, 2014a). To date, diverse types of VOCs have been detected in the atmosphere with concentrations in the order of μg/m<sup>3</sup> of air. Typical nonpolar VOCs include aliphatic compounds (e.g., methane, hexane, heptane), halogenated hydrocarbons (e.g., chloroform, dichloromethane, dichloroethane, trichloroethene, trichloroethylene, carbon tetrachloride, chlorobenzene, and dichlorobenzenes), and aromatic compounds. Among the aromatic compounds, 60–90% are detected in the atmosphere as benzene, toluene, xylenes, ethylbenzene, and 1,2,4-trimethylbenzene (Jang et al., 2004; Arp et al., 2008a; Matsumoto et al., 2010). Typical polar VOCs include acetone, ethyl acetate, methyl isobutyl ketone, butyl acetate, ethanol, propanol,

isopropanol, and dioxanes, to name a few. These VOCs contain hydrophilic functional groups including hydroxyl, carbonyl, and ether groups (Jang et al., 2004; Odabasi et al., 2005; Arp et al., 2008a; Matsumoto et al., 2010).

Many VOCs are toxic. Inhaled VOCs have been linked to irritation of eye, nose, and throat, headaches, loss of coordination, nausea, damage of liver, kidney, and central nervous system, and hematological problems (US EPA, 2014b). VOCs such as benzene, 1,3-butadiene, and formaldehyde can cause cancer and/or leukemia in humans (Seitz and Stickel, 2010; St.Helen et al., 2014). Other VOCs such as methylene chloride, perchloroethylene, naphthalene, paradichlorobenzene, chloroform, and acetaldehyde can induce cancer in animals and are suspected carcinogens in humans (Seitz and Stickel, 2010; St.Helen et al., 2014; US EPA, 2014b).

Although it is important to understand the partitioning of VOCs into aerosols, only scant reports exist about the mechanism and the extent of partitioning. In contrast, over the past decades, the partitioning of SVOCs (e.g., polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), polychlorinated dibenzo-*p*-dioxins/furans (PCDD/Fs)) into aerosols has been extensively studied (Fig. 1) because of their higher extent to partition into aerosols and higher measurability than VOCs. The partitioning behavior of some SVOCs have been used as surrogates to estimate VOC/aerosol partitioning. However, SVOCs have physicochemical properties that substantially differ from VOCs, thus using SVOCs to approximate the behavior of VOCs may not fully account the VOC/aerosol partitioning mechanism.

SVOCs are typically nonpolar or weakly polar with large

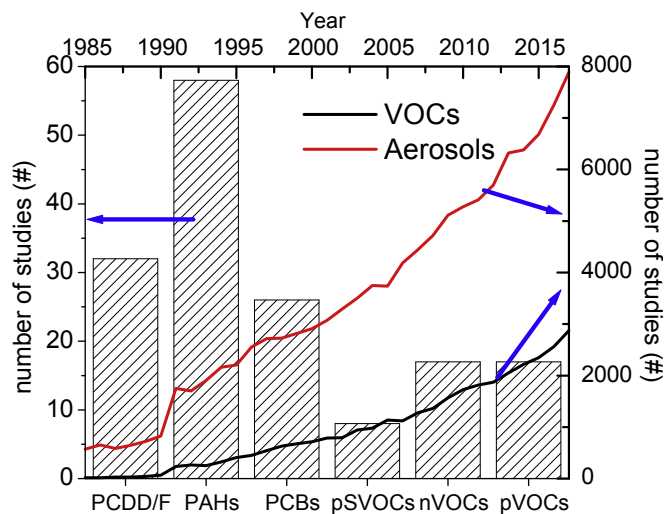


Fig. 1. Number of papers published on VOCs and aerosols (red and black curves), and gas-to-particle partitioning for nonpolar SVOCs (PCDD/F, PAHs, PCBs), polar SVOCs (pSVOCs), nonpolar VOCs (nVOCs), and polar VOCs (pVOCs) (column bars) in Web of Science from 1985 to 2017.

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