|  |
| --- |
| Predicting and Parameterizing the Glass Transition Temperature of Atmospheric Organic Compounds via Molecular Dynamics Simulations**Panagiota Siachouli,**1,#, **Vlasis G. Mavrantzas**1,2,3,\* and **Spyros N. Pandis**1,2,\*1 Department of Chemical Engineering, University of Patras, Patras, GR 26504, Greece.2 Institute of Chemical Engineering Sciences (ICE-HT/FORTH), Patras, GR 26504, Greece.3 Particle Technology Laboratory, Department of Mechanical and Process Engineering, ETH Zürich, CH-8092 Zürich, Switzerland.# Presenting author: Panagiota Siachouli, email: nota.siachouli@hotmail.com\* Corresponding authors: Vlasis G. Mavrantzas, email: vlasis@chemeng.upatras.gr , Spyros N. Pandis, email: spyros@chemeng.upatras.gr  |

abstract

Aerosols, typically defined as suspended liquid or solid particles in Earth’s atmosphere, are ubiquitous. Atmospheric particulate matter contains thousands of complex organic compounds, most of which remain unidentified. To understand and categorize these compounds, exploring their physicochemical properties and phase state is essential. The glass transition temperature (Tg) is a crucial property that provides insight into their phase state, marking the transition between a more fluid, rubbery state and a brittle, glassy state. Deciphering the phase state of organic compounds is critical for understanding various atmospheric processes. In particular, a solid or glassy phase state can potentially reduce the rate of heterogeneous chemical reactions, inhibit water uptake, alter the atmospheric lifetime of particles, and influence their long-range transport.[1]

Despite its importance, experimentally investigating Tg is a daunting task due to difficulties in the synthesis and purification of the compounds. Furthermore, Tg is highly sensitive to the thermal history of the system under study and the protocols used to extract the measurement. Both factors are often unknown, thereby making it difficult to verify and reproduce results.[2] To this end, we employ Molecular Dynamic Simulations (MD) to investigate the Tg of pure, atmospherically relevant, organic compounds. MD simulations can bypass the difficulties encountered in experimental studies; simultaneously, they offer detailed insights at the molecular level, thus rendering them a valuable tool for understanding physicochemical properties.

This work curates a comprehensive dataset of glass transition temperatures for organic compounds, considering factors such as number of carbon atoms, types of functional groups present and their coexistence, and molecular architecture. The molecular weight and oxygen to carbon ratio (O:C) are also taken into account.[3] The compiled dataset is used to create a parameterization for the Tg which incorporates these factors, including carbon and oxygen atoms, functional groups and the architecture (linear/ring-like) and indirectly the molecular weight and O:C ratio. The parameterization enables the generalization of the MD results and contributes to the more accurate prediction of Tg, which can enhance our understanding of the behavior of organic aerosols and improve climate model predictions.

**REFERENCES**

[1] N.E. Rothfuss and M.D. Petters. 2017. *Environ. Sci. Technol*., **51**, 271-279.

[2] O.V. Mazurin and Yu Gankin. 2004. *Journal of non-crystalline solids,***342:** 166-169.

[3] P. Siachouli, K.S. Karadima, V.G. Mavrantzas, S.N. Pandis. 2024. *Soft Matter,***20:** 4783-4794.