Cyprus University of Technology

Faculty of Geotechnical Sciences and Environmental Management

Doctoral Dissertation

WATER-SALT-ORGANIC INTERACTIONS WITHIN ATMOSPHERIC AEROSOL: A MOLECULAR DYNAMICS STUDY

Anastasia Salameh

Limassol, March 2021

CYPRUS UNIVERSITY OF TECHNOLOGY

FACULTY OF GEOTECHNICAL SCIENCES AND ENVIRONMENTAL MANAGEMENT

DEPARTMENT OF CHEMICAL ENGINEERING

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Approval Form

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“To my father, in loving memory”

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PUBLICATIONS

This thesis is based in part on the following articles prepared during the research project:

I. Correlation between Surface Tension and the Bulk Dynamics in Salty Atmospheric Aquatic Droplets

Authors: Anastasia Salameh, Flora Vorka, Vangelis Daskalakis

Publication: The Journal of Physical Chemistry C

Publisher: American Chemical Society

Date: Jun 1, 2016

II. Atmospheric Ice Nucleation by Glassy Organic Compounds: A Review

Authors: Anastasia Salameh, Vangelis Daskalakis

Publication: Chemistry of Compounds Journal

Publisher: Verizona Open Access (CCJ-Journal)

Date: Feb 6, 2017

ABSTRACT

This thesis's focal point is to advance our knowledge regarding the interactions between water, salt, and organics in the atmosphere, with applications in ice nucleation and cloud condensation nuclei (CCN) formation. This knowledge can be employed in the future for atmospheric modeling. High in the clouds, water molecules transition into ice crystals within particles composed of a mix of sea salt and organic materials. These crystals are significant players in the generation of rain and snow, controlling the balance between heating and cooling the planet by scattering the sunlight. The particles that seed ice crystals are swirled into the atmosphere from both land and sea. But only a few particles can act as a nucleus for forming ice crystals or condensation nuclei, making them more effective ice/ cloud nucleators. This suggests that the few particles that do seed or nucleate ice crystals have specific physical or chemical properties. Ice nucleation is a crucial step in cloud formation and precipitation and plays an important role in the Earth's hydrological cycle, energy balance, and radiative balance. Given its significance, atmospheric ice/cloud nucleation on organic and salt aerosol particles is one of the microscopic processes that are still poorly understood. Significant uncertainties exist in the representation of nucleation processes in climate models. Therefore, probing aqueous organic and salt aerosol particles is a challenge. This opens the door for computer simulations and modeling of these intricate structures. The work presented herein probes these processes by employing molecular dynamic simulations to understand the impacts of aerosol-cloud interactions and atmospheric chemistry.

Keywords: water, atmospheric ice nucleation, salts, organics, molecular dynamics, simulations