RGC Ref.: M-HKUST609/12
(please insert ref. above)

The Research Grants Council of Hong Kong
SRFDP & RGC ERG Joint Research Scheme
Completion Report

(Please attach a copy of the completion report submitted to the Ministry of Education by the Mainland researcher)

Part A: The Project and Investigator(s)

1. Project Title

Chemical Speciation and Source Identification of Water-soluble Organic Aerosols in Urban Environments for a Mechanistic Understanding of Haze Pollution
基于霾污染机制的复合型城市大气颗粒物中水溶性有机碳的种态与来源

2. Investigator(s) and Academic Department/Units Involved

	Hong Kong Team	Mainland Team
Name of Principal Investigator *(with title)*	Jianzhen Yu	Guangli XIU
Post	Professor	Professor
Unit / Department / Institution	Department of Chemistry and Division of Environment/ HKUST	School of Resources & Environment Engineering/ East China University of Science & Technology
Contact Information	chjianyu@ust.hk 852-2358-7389	xiugl@ecust.edu.cn 86-133-1186-9510
Co-investigator(s) *(with title and Institution)*		
PhD student(s) (with period of involvement)	Name: 1) WU Cheng 2) KUANG Binyu 3) LI Yugen 4) WANG Nijing+ Institution: HKUST Period from 1) and 2) 1 Mar. 2013-29 Feb. 2016 3) 1 Feb. 2015-31 Dec. 2016 4) 1 Sep. 2015-31 Jul. 2016	Name: 1) XU Wei 2) LEI Xiaoning 3) HUANG Zhongsi+ 4) QIAO Ting+ 5) LI Bo+ 6) ZHAO Mengfei+ Institution: ECUST Period from: 1 Mar. 2013-29 Feb. 2016 +: Master students

Note: The Hong Kong project team must involve at least one research postgraduate student pursuing a Doctor of Philosophy degree at the UGC-funded university (PhD student) at any time throughout the project period.

3. Project Duration

	Original	Revised	Date of RGC/ Institution Approval *(must be quoted)*
Project Start date	1 Mar. 2013		
Project Completion date	29 Feb. 2016		
Duration *(in month)*	36		
Deadline for Submission of Completion Report	28 Feb. 2017		

Part B: The Completion Report

5. Project Objectives

5.1 Objectives as per original application

1. To obtain data on the chemical speciation and size distribution characteristics of water-soluble organic aerosols in the urban atmospheres of Hong Kong and Shanghai.
2. To determine the relative abundance of water-soluble inorganic ions and organic carbon for the assessment of relative contributions to haze pollution by the two.
3. To identify and apportion major sources of water-soluble organic aerosols in Hong Kong and Shanghai and to assess the relative contributions of primary and secondary sources.
4. To establish an empirical relationship between light extinction by aerosol and major aerosol constituents, including water-soluble organic carbon species.

5.2 Revised Objectives

Date of approval from the RGC: _____

Reasons for the change: _____
_____

1.
2.
3. ....

Not Applicable

6. Research Outcome

Major findings and research outcome
(maximum 1 page; please make reference to Part C where necessary)

Haze pollution is known to be associated with high levels of particulate matter (PM). As such, it is vital to establish the quantitative link between visibility degradation and individual components of PM. IMPROVE formula is an empirical equation established in the US through decades of nationwide monitoring efforts of both optical properties and chemical composition. However, the applicability of this formula cannot be assumed for the more heavily polluted urban environments in China. When using the IMPROVE formula to reconstruct light extinction from measured PM components, we showed through this project that the IMPROVE formula underestimates the measured data by ~20% for the light scattering coefficient and ~10% for the light absorbing coefficient. We further developed our local empirical formula which explains well the observed light extinction values. The underestimation was revealed to be due to inaccurate representation of organic carbon (OC) contributions to both light scattering and absorption in the IMPROVE formula (Li et al., 2017a).

Our research is the first effort to examine the mass scattering and absorption efficiencies (MSE and MAE) of specific organic carbon components separated by water solubility or water affinity. This is possible with our speciated measurements of the water-soluble (OC) into hydrophobic and hydrophilic parts (Wang and Yu, 2017). We have shown that the localized formulas yield similar MSEs for the inorganic components to those in the original IMPROVE equation. In comparison, the MSE for OC derived in the local formulas is significantly larger than that in the IMPROVE formula, explaining the underestimation of the measured light scattering coefficient by the IMPROVE formula. Within organic matter, the hydrophilic part is found to have a stronger ability (i.e., higher MSE) to attenuate light than the hydrophobic part on a per carbon mass basis (Li et al., 2017a). This result represents a significant advance in improving our predictive capability for light extinction due to PM components.

We further coupled receptor modeling with light extinction data to apportion light extinction to significant pollution sources and developed a set of formulas to calculate light extinction by aerosol sources (Li et al., 2017b). Such formulas could be easily adopted by policy-makers to evaluate impact on visibility of source-specific intervention measures.

On more fundamental aspects, we investigated the dependence of liquid water content (LWC) taken up by PM on ionic chemical composition, particularly on the relative abundance of sulfate and nitrate (Xue et al., 2014). LWC contributes significantly to PM's ability for haze-formation, as its mass could even exceed the dry PM mass under humid conditions. Through examining a historical data set of 520 half-hourly measurements of ionic chemical composition in $PM_{2.5}$ at a receptor site in Hong Kong, we showed that LWC would increase by ~15-200% (depending on relative humidity) if half of the current sulfate is replaced by nitrate. Such a scenario analysis is relevant to the trend of reducing SO_2 while increasing in NOx emission.

In current urban atmospheric environments in China, sulfate largely remains to be the single most significant water-soluble PM component and is often significantly enhanced during pollution episodes. We used an observation-based model for secondary inorganic aerosols to simulate sulfate formation pathways under conditions of haze-fog events encountered in Chinese megacities (Xue et al., 2016). The model analysis identified, at a typical haze-fogwater pH of 5.6, the most important pathway was oxidation of S(IV) by dissolved NO_2, followed by the heterogeneous reaction of SO_2 on the aerosol surface. The model results indicate that the unique cocktail of high fogwater pH, high concentrations of NO_2, SO_2, and PM, and small fog droplets is capable of greatly enhancing sulfate formation. Such haze-fog conditions could lead to rapid sulfate production at night and subsequently high $PM_{2.5}$ in the morning when the fog evaporates. Sulfate formation is simulated to be highly sensitive to fogwater pH, PM, and precursor gases NO_2 and SO_2. Such insights on major contributing factors imply that reduction of road dust and NOx emissions could lessen $PM_{2.5}$ loadings and haze formation in Chinese megacities during fog events.

Potential for further development of the research and the proposed course of action
(maximum half a page)

The local empirical formula, considering speciation of the organic carbon into hydrophobic and hydrophilic components, is inherently more robust than the original IMPROVE formula. Repeating the same suite of chemical and optical measurements in an urban environment very different from that in Hong Kong will allow us to evaluate the general applicability of the formula. Through this project, we found that visibility sensor measurements are not ideally representing the ability of light extinction by PM. For the study of the linkage of visibility and PM, it is necessary to use more reliable optical properties, such as those provided by nephelometers and aethalometers. Inspired by the findings from this project, we are developing research proposals to further improve our ability to predict visibility degradation.

7. The Layman's Summary

(describe in layman's language the nature, significance and value of the research project, in no more than 200 words)

Haze pollution, characterized by high particulate matter (PM), is becoming increasingly serious in Hong Kong and many urban areas in China. The primary cause of poor visibility is the small particles suspended in the atmosphere, also called $PM_{2.5}$. The water-soluble components in $PM_{2.5,}$ including inorganic ions and water-soluble organic carbon (WSOC) species, could exacerbate light extinction through their ability to take up water vapor from the surrounding ambient atmosphere. We have a reasonable understanding of the contribution of inorganic ions to visibility degradation, but we know little about the link between WSOC and visibility. WSOC could either suppress or enhance water uptake by inorganics in atmospheric PM, depending on the chemical make-up of the WSOC fraction. In this project, we separated WSOC aerosols into hydrophilic and hydrophobic fractions and quantified them along with inorganic ions. This allowed us to develop a more robust empirical formula to link PM chemical components with light extinction. A high light extinction mass efficiency was determined for the hydrophilic part of OC. Such a formula provides an improved tool for modelers and policymakers to predict visibility degradation from individual chemical components or individual aerosol sources.

Part C: Research Output

8. Peer-reviewed journal publication(s) arising directly from this research project

(Please attach a copy of each publication and/or the letter of acceptance if not yet submitted in the previous progress report(s). All listed publications must acknowledge RGC's funding support by quoting the specific grant reference.))

The Latest Status of Publications				Author(s) ***(bold** the authors belonging to the project teams and denote the corresponding author with an asterisk*)*	Title and Journal/ Book *(with the volume, pages and other necessary publishing details specified)*	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
Year of publication	Year of Acceptance *(For paper accepted but not yet published)*	Under Review	Under Preparation *(optional)*						
2014				Jian Xue, **Stephen M. Griffith**, Xin Yu, Alexis K. H. Lau, **Jian Zhen Yu***	Effect of nitrate and sulfate relative abundance in PM2.5 on liquid water content explored through half-hourly observations of inorganic soluble aerosols at a polluted receptor site, *Atmospheric Environment*, 2004, v99, 24-31.	2014	no	yes	yes
2016				Jian Xue, Zibing Yuan, **Stephen M. Griffith**, Xin Yu, Alexis K. H. Lau, **Jian Zhen Yu***	Sulfate Formation Enhanced by a Cocktail of High NOx, SO_2, Particulate Matter, and Droplet pH during Haze-Fog Events in Megacities in China: An Observation-Based Modeling Investigation. *Environmental Science & Technology*, *50*(14), 7325-7334.	2017	yes	yes	yes
2017				**Yugen Li**, **H.H. Hilda Huang, Stephen M. Griffith, Cheng Wu**, Alexis K. H. Lau, & **Jian Zhen Yu***	Quantifying the relationship between visibility degradation and PM 2.5 constituents at a suburban site in Hong Kong: Differentiating contributions from hydrophilic and hydrophobic organic compounds. *Science of the Total Environment*, *575*, 1571-1581	2017	yes	yes	yes
		2017		**Nijing Wang, Jian Zhen Yu***	Size Distributions of Hydrophilic and Hydrophobic Fractions of Water-Soluble Organic Carbon in an Urban Atmosphere. Submitted to *Atmospheric Environment*.	2017	no	yes	no‡
			2017	**Yugen Li**, **Stephen M. Griffith, H.H. Hilda Huang, Cheng Wu**, Alexis K. H. Lau, & **Jian Zhen Yu***	Source apportioning of light extinction coefficient at a suburban site in Hong Kong, to be submitted to *Atmospheric Environment*.	2017	no	yes	no‡

‡ These two papers will be deposited in the institutional repository once they have been through the peer-review process.

9. Recognized international conference(s) in which paper(s) related to this research project was/were delivered *(Please attach a copy of each delivered paper. All listed papers must acknowledge RGC's funding support by quoting the specific grant reference.)*

Month/Year/ Place	Title	Conference Name	Submitted to RGC *(indicate the year ending of the relevant progress report)*	Attached to this report *(Yes or No)*	Acknowledged the support of this Joint Research Scheme *(Yes or No)*	Accessible from the institutional repository *(Yes or No)*
04/2014	Size Distribution of Urban Aerosol Carbon Composition in Tsuen Wan, HK: Organic Carbon, Water-Soluble Organic Carbon and Carbon in Humic-Like Substances	The 21th Symposium on Chemistry Postgraduate Research in Hong Kong	2014	No	Yes	Yes
05/2014	Size Distribution Characteristics of Organosulfates in Humic-like Substances in the Pearl River Delta Region	The 7th World Congress on Particle Technology	2014	No	Oral acknowledgement	Yes
04/2017	Quantifying the relationship between visibility degradation and PM2.5 constituents at a suburban site in Hong Kong: Differentiating contributions from hydrophilic and hydrophobic organic compounds	European Geosciences Union General Assembly 2017, Vienna, Austria, 23-28, 2017	2017	Yes	Yes	No‡

‡ The conference paper will be deposited in the institutional repository once the final conference proceeding is available.

10. Student(s) trained *(Please attach a copy of the title page of the thesis.)*

Name	Degree registered for	Date of registration	Date of thesis submission/ graduation
Cheng WU	PhD in Atmospheric Environmental Science	Jan. 2010	Jan. 2015
Binyu KUANG	PhD in Chemistry	1 Sep. 2011 as a MPhil 1 Sep. 2013 as a PhD	Jan. 2017
Nijing WANG	MPhil in Technology Leadership & Entrepreneurship	1 Sep. 2013	Aug. 2015
Yugen LI	PhD in Environmental Sci. Policy & Management	1 Feb. 2015 as a MPhil 1 Sep. 2016 as a PhD	Aug. 2019

11. Other impact *(e.g. award of patents or prizes, collaboration with other research institutions, technology transfer, etc.)*

Collaboration with Prof. Dui WU's group in Jinan University has been established as a result of this research work. We are collaborating in developing a research proposal to extend the examination of optical and chemical data to a Guangzhou urban location.