Modeling of Ground-level Ozone Formation in Urban Air-sheds of Sri Lanka

Doctor of Philosophy Thesis

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by

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May 2022

DECLARATION

The work submitted in this dissertation is the result of my own investigation, except where otherwise stated.

It has not already been accepted for any degree, and is also not being concurrently submitted for any other degree.

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Gamage Bimalka Sajeevi Perera

Date:……

We endorse the declaration by the candidate.

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ABSTRACT

Physical phenomenon of the relation among ground-level ozone (O_3), oxides of nitrogen (NO_X) and volatile organic compounds (VOC) is governed by complex nonlinear photochemistry. To predict and control O_3 concentration, it is vital to know, how O_3 concentration changes in response to prescribed changes in source emissions of NO_X and VOCs. In this research, a theoretical model was developed and validated for ground-level O_3 formation in urban air-sheds of Sri Lanka. Hourly averaged weekly results of ambient pollutant concentration data of eleven cities in the base years 2013, 2014 and 2015 in Sri Lanka was assessed and an urban air shed model was developed. The model was calibrated using influential parameters measured. Then Colombo as the most complicated urban air-shed in Sri Lanka was analyzed in detail. Model was validated using measured 24-hour air quality monitoring data from the mobile air quality monitoring stations at major traffic locations in Colombo in the year 2018 and 2019. Operational schedules of emission sources including train scheduled data, working hours of the thermal power plants, and vehicle counts were conducted at identified critical locations in Colombo to investigate the responsible sources. Gases from the exhaust line of different types of vehicles was collected and analyzed using Gas Chromatography Mass Spectroscopy (GCMS).

Results confirm that there exist two regimes of NO_X-VOC-O_3 sensitivity as NO_x-sensitive regime and VOC-sensitive regime. The urban air-shed model is capable of estimating the ground-level steady state ozone concentration (O_{3ss}) and contributions from each regime. The univariate linear regression model using predicted and observed O_3 values confirmed that O_{3ss} concentration was significantly correlated with the predicted O_3 concentration. Analysis of urban air shed in Colombo also confirms the predicted and observed O_{3ss} concentration were significantly correlated. This research provides a detailed understanding of photochemical degradation on formation of ground-level O_3 in urban air-sheds of Sri Lanka and provides critical information for the scientific community and decision-makers to formulate air pollution mitigation policies.

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LIST OF ABBREVIATIONS

AEA	Atomic Energy Authority
AirMAC	Air Resource Management Centre
ATS	American Thoracic Society
CAI-Asia	Clean Air Initiatives in Asia
CB4	Carbon Bond Mechanism 4
CB5	Carbon Bond Mechanism 5
CEA	Central Environmental Authority
CEB	Ceylon Electricity Board
CFC-11 (CCl_3F)	Chlorofluorocarbons
CFC-12 (CCl_2F_2)	Chlorofluorocarbons
CNG	Compact Natural Gas
CH_3CN	Methyl Cyanide
CH_4	Methane
CMC	Colombo Municipal Council
CO	Carbon monoxide
CO_2	Carbon dioxide
°C	Celsius
COPD	Chronic obstructive pulmonary disease
DMT	Department of Motor Traffic
FID	Flame Ionization Detection
FIDs	Flame Ionization Detectors
FSRU	Floating Storage Regasification Unit
FT	Free troposphere
GC	Gas Chromatograph

GCMS	Gas Chromatograph/Mass Spectrometer
GHG's	Greenhouse Gases
GOSL	Government of Sri Lanka
GWP	Global warming potential
HCHO	Formaldehyde
HCN	Hydrogen Cyanide
HEI	Health Effects Institute
HO_2	Hydro-peroxy radicals
IAP	Indoor air pollution
IARC	International Agency for Research on Cancer
IPCC	Intergovernmental Panel on Climate Change
IT	Interim targets
ITI	Industrial Technology Institute
JICA	Japan International Cooperation Agency
LRT	Light Rail Transport
LNG	Liquid Natural Gas
LPG	Liquid Petroleum Gas
MCM	Master Chemical Mechanism
MIM	Mainz Isoprene Mechanism
MW	Mega Watt
$\mu g/m^3$	Micro gram for cubic meter
μm	Micro meter
mm	Mile meter
MOF	Ministry of Finance
MTBE	Methyl Tertiary Butyl Ether

N_2	Nitrogen
N_2O	Nitrous oxide
N_2O_5	Dinitrogen pentoxide
NBRO	National Building Research Organization
NEA	National Environmental Act
NH_3	Ammonia
NO	Nitrogen oxide
NO_2	Nitrogen dioxide
NO_3	Nitrate radical
NOU	National Ozone Unit
NO_X	Oxides of nitrogen
O(1D)	Excited oxygen atom
O(3P)	Ground state oxygen atom
O_2	Oxygen
O_3	Ozone
OH	Hydroxyl radical
OVMs	Organic Vapour Monitors
OVOCs	Oxygenated Volatile Organic Compounds
PBL	Planetary Boundary Layer
PCBs	Polychlorinated biphenyls
PID	Photo Ionization Detection
PIDs	Photo-Ionization Detectors
PM	Particulate matter
PM_{10}	Particulate matter less than 10 microns (µm) in diameter
$PM_{2.5}$	Particulate matter less than 2.5 microns (µm) in diameter

POCP	Photochemical Ozone Creation Potentials
POPs	Persistent Organic Pollutants
PPCP	Photochemical PAN Creation Potentials
ppm	Parts per million
pptv	Parts-per-trillions by volume
PTR-MS	Proton-transfer-reaction mass spectrometry
R	Alkyl radical
RACM	Regional Atmospheric Chemistry Mechanism
RO	Alkoxy radical
RO_2	Peroxy radicals
RPM	Respirable Particulate Matter
RTS	Rapid Transit System
SAPRC	Statewide Air Pollution Research Centre
SEI	Stockholm Environment Institute
SLAQI	Sri Lanka Air Quality Index
SLVET	Sri Lanka vehicle emission testing program
SMEs	Small and Medium Enterprises
SO_2	Sulfur dioxide
SOA	Secondary organic aerosols
SPM	Suspended Particulate Matter
SVOCs	Semi Volatile Organic Compounds
TSP	Total Suspended Particulates
UK	United Kingdom
UNEP	United Nations Environment Programme
USA	United States America

USEPA	United States Environmental Protection Agency
UV	Ultra-Violet
VOC	Volatile Organic Compound
VOCs	Volatile Organic Compounds
VOHAPs	Volatile Organic Hazardous Air Pollutants
vol/vol	Volume to volume
VVOCs	Very Volatile Organic Compounds
WHO	World Health Organization
WRMPPP	Western Region Mega Polis Plan