

MODELLING OF TROPOSPHERIC OZONE AND SOURCE- SPECIE APPORTIONMENT IN AN URBAN AREA

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MODELLING OF TROPOSPHERIC OZONE AND SOURCE-SPECIE APPORTIONMENT IN AN URBAN AREA

by

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DEDICATED

TO

MY FAMILY AND FRIENDS

Certificate

This is to certify that the thesis entitled “**Modelling of tropospheric ozone and source-specie apportionment in an urban area**”, being submitted by **Mr. Sumit Sharma**, to the Indian Institute of Technology Delhi for the award of ‘**Doctor of Philosophy**’ in Department of Civil Engineering is a record of the bonafide research work carried out by him under my supervision and guidance. He has fulfilled the requirements for the submission of this thesis, which to the best of my knowledge has reached the requisite standard.

The material contained in the thesis has not been submitted in part or full to any other University or Institute for the award of any other degree or diploma.

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Abstract

Ozone is a pollutant of concern at many places across the world, even in the developed countries. Indian sub-continent shows high values of ozone, which can have significant impacts over human health, crop productivity and regional scale climatic patterns. Ozone, being a secondary pollutant, is formed by reactions of pollutants like NO_x, CO and VOCs, in the presence of sunlight. Considering non-linear chemistry of ozone with the precursor pollutants, apportionment of sources and species responsible for its formation is a challenging but important task. There are action plans in place for control of PM pollution in different cities in India, however, there exists limited research studies for understanding the causal factors for O₃ formation and its control in India. This study has aimed at modelling of ground level ozone concentrations in an urban setting and carrying out the source-specie apportionment to understand causal relationships. The study also analyses the roles played by different precursor species (NO_x and VOCs) in formation of ozone in a typical urban region.

Preliminary analysis of monitored data of ozone in Delhi shows that there are episodes of high ozone levels during specific days and seasons. The assessment of statistical distribution of ozone data has revealed that it broadly follows the 3-parameter lognormal distribution model, except in autumn where Weibull distribution is detected. This suggests longish tail of the distribution mainly on account of high ozone concentration episodes, especially during enhanced photo-chemical activity. Preliminary model runs with an existing inventory of precursors have shown satisfactory performance of CMAQ model for prediction of ozone concentrations in Delhi for the year 2010. Further, it has been found that the performance improves with the use of a hybrid model based on concatenation of outputs from deterministic (CMAQ) model and statistical distribution models. Based on the satisfactory performance of the CMAQ model in the preliminary analysis, it has been chosen for detailed modelling and source-specie apportionment of ozone concentrations in a wider Delhi-National Capital Region

(Delhi-NCR). Detailed high-resolution multi-sectoral inventories have been developed for the Delhi-NCR for the year 2012. The inventories have shown that transport sector accounts for 55% of the total NO_x emissions, followed by power plants (23%) and DG sets (7%). In NMVOC inventories, transport sector again accounts for 33%, followed by evaporative emissions released from solvent use and fuel handling activities (30%), and agricultural residue burning (28%). Meteorological model runs were performed using the WRF model for the year 2012. Validated outputs of WRF, in the form of 3-dimensional meteorological fields, have been fed into the CMAQ model for prediction of ozone concentrations using detailed emission inventories. Model performance has been evaluated on a variety of evaluation metrics and has been found to be satisfactory. The modelled monthly average ozone concentrations in the overall study domain (NCR) have varied between 78-114 $\mu\text{g}/\text{m}^3$ (98 $\mu\text{g}/\text{m}^3$ average) across different months; while within the city of Delhi the concentrations are lower and vary between 56-98 $\mu\text{g}/\text{m}^3$ (average 76 $\mu\text{g}/\text{m}^3$), mainly due to titration effect. Further, simulations using ISAM-CMAQ have been carried out for the whole year 2012 to ascertain the grid-wise source contributions based on the two ozone formation regimes (NO_x or VOC sensitive). Evaluations carried out at a monthly averaged basis show that the share of boundary conditions i.e. contributions from outside of the domain, is prominent all across the year in NCR. The share of boundary conditions (BC) is about 92-93%, 88-92%, and 87-89% in whole NCR, Delhi, and at a downwind location to Delhi, respectively. However, the share of local sources becomes important, when analysed at an hourly averaged scale. The maximum contribution of local sources in hourly ozone concentrations in Delhi goes up to 46% in summers, and upto 26% in winters. Among these local sources, the major contributors are transport (13-31%), power generation (2-10%), non-energy sources (1-3%), and neighbouring region sources (2-8%). The downwind location to the Delhi city has shown even higher contribution of local sources, reaching up to 56% in the post-monsoon season. This was due to atmospheric transport of ozone

and its precursors from Delhi to downwind regions. It has been concluded that while regional contributions are significantly high in NCR, the local source contributions are very important during certain episodes, mainly during high photo-chemical activity. Conclusively, control measures are required for local as well as regional contributors. Comparing the two ozone formation regimes, the contribution of NO_x limited regime is found to be higher in the summer months, mainly due to low NO_x/VOC ratios. In winters, biogenic VOC emissions are low and higher NO_x/VOC ratios are prevalent which lead to development of VOC limited conditions. The share of VOC limited conditions in ozone formed in Delhi goes up from 12% in June to 55% in December depicting a shift from NO_x limited to VOC limited conditions from summers to winter seasons, respectively.

Excluding the contributions of boundary conditions at the downwind location to Delhi, transport sector contributes to 49-65% of locally formed ozone in NO_x limited regime, followed by power (12-21%), while in the VOC limited regime, transport sector contributes to 39-66% in ozone followed by 7-22% contributions from evaporative sources and open agricultural burning contributing up to 34% in some months. The share of VOC limited conditions in ozone formed in downwind regions of Delhi goes up from 14% in June to 65% in December.

This study successfully demonstrates the use of photo-chemical transport models to predict ozone concentrations in an urban setting in India. The study also shows the results of source-specie apportionment of ozone in Delhi-NCR, which can also be used for scenario development and policy analysis for evaluating local and regional scale interventions for control of ozone.

सार

ओजोन दुनिया भर के कई स्थानों पर, यहां तक कि विकसित देशों में भी, चिंता का विषय है, । भारतीय उपमहाद्वीप ओजोन का उच्च स्तर दर्शाता है, जो मानव स्वास्थ्य, फसल उत्पादकता और क्षेत्रीय पैमाने पर जलवायु पर महत्वपूर्ण प्रभाव डाल सकता है। ओजोन, एक माध्यमिक प्रदूषक होने के नाते, सूरज की रोशनी की उपस्थिति में, नाइट्रोजन के आक्साइड (नाकॅस), कार्बन मोनोऑक्साइड, और वीओसी जैसे प्रदूषकों की रासायनिक प्रतिक्रिया द्वारा उत्पन्न होती है । पूर्ववर्ती प्रदूषकों के साथ ओजोन की गैर-रैखिक संबंध को ध्यान में रखते हुए, इसके उत्पत्ति के लिए जिम्मेदार स्रोतों और प्रदूषकों का मूल्यांकन एक चुनौतीपूर्ण लेकिन महत्वपूर्ण कार्य है। भारत में शहरों में प्रदूषण नियंत्रण के लिए कई योजनाएं हैं, परंतु ओजोन और उसके नियंत्रण के तरीके को समझने के लिए सीमित शोध अध्ययन मौजूद हैं। इस अध्ययन का उद्देश्य शहरों में जमीनी स्तर पर ओजोन सांद्रता की मॉडलिंग और इसके उत्पत्ति के लिए जिम्मेदार स्रोतों और प्रदूषकों का मूल्यांकन करना है। अध्ययन में एक विशिष्ट शहरी क्षेत्र में ओजोन के उत्पत्ति में विभिन्न प्रदूषकों (एनओएक्स और वीओसी) द्वारा निभाई गई भूमिकाओं का भी विश्लेषण किया गया है।

दिल्ली में ओजोन के आंकड़ों के प्रारंभिक विश्लेषण से पता चलता है कि विशिष्ट दिनों और मौसमों के दौरान ओजोन का स्तर उच्च होता है । ओजोन डेटा के सांख्यिकीय वितरण के आकलन से पता चला है कि यह मोटे तौर पर 3-पैरामीटर लॉगनॉर्मल डिस्ट्रीब्यूशन मॉडल का अनुसरण करता है; केवल शरद ऋतु में वेइबुल डिस्ट्रीब्यूशन मॉडल देखा गया है । प्रारंभिक विश्लेषण के लिए, सी.एम.ए.क्यू .मॉडल को एक मौजूदा प्रदूषक उत्सर्जन इन्वेंट्री डेटाबेस के साथ चलाया गया, जो वर्ष २०१० में दिल्ली में ओजोन सांद्रता के पूर्वानुमान के लिए संतोषजनक प्रदर्शन दिखाता है। इसके अलावा, यह पाया गया है कि एक संकर मॉडल (निर्धारक सी.एम.ए.क्यू .मॉडल और सांख्यिकीय वितरण मॉडल के संयोजन द्वारा बनाया गया) के उपयोग के साथ प्रदर्शन में और सुधार होता है। प्रारंभिक विश्लेषण में सी.एम.ए.क्यू. मॉडल के संतोषजनक प्रदर्शन के आधार पर, इस मॉडल को दिल्ली-राष्ट्रीय राजधानी क्षेत्र (दिल्ली-एनसीआर) में विस्तृत मॉडलिंग और ओजोन सांद्रता की उत्पत्ति में विभिन्न स्रोतों और प्रदूषकों द्वारा निभाई गई भूमिकाओं के विश्लेषण के लिए चुना गया । वर्ष

२०१२ के लिए दिल्ली-एनसीआर के लिए विस्तृत, उच्च-रिज़ॉल्यूशन, बहु-क्षेत्रीय, प्रदूषक इन्वेंट्री विकसित की गई। इनवेंट्री से पता चला है कि ट्रांसपोर्ट सेक्टर में कुल नॉक्स उत्सर्जन का ५५% हिस्सा है, उसके बाद बिजली संयंत्र (२३%) और डीजी सेट (७%) हैं। एनएमवीओसी इन्वेंट्री में, ट्रांसपोर्ट सेक्टर की फिर से ३३% हिस्सेदारी है, जिसके बाद विलायक उपयोग और ईंधन वितरण की गतिविधियों (३०%), और कृषि अवशेषों (२८%) का हिस्सा है। मौसम संबंधी मॉडलिंग वर्ष २०१२ के लिए मौसम अनुसंधान पूर्वानुमान (डबलयु. आर. एफ.) मॉडल का उपयोग किया गया।

विस्तृत उत्सर्जन प्रदूषक इन्वेंट्री का उपयोग करते हुए, ओजोन सांद्रता के पूर्वानुमान के लिए, ३-आयामी डबलयु. आर. एफ. मॉडलिंग के आउटपुट को सी.एम.ए.क्यू मॉडल में डाला गया। विभिन्न प्रदर्शन मूल्यांकन मीट्रिक पर मॉडल का मूल्यांकन किया गया और इसे संतोषजनक पाया गया। एनसीआर में मासिक औसत ओजोन सांद्रता विभिन्न महीनों में ७८-११४ माइक्रोग्राम प्रति घन मीटर (९८ औसत) के बीच पायी गयी है। मुख्यतः अनुमापन रसायन विज्ञान (टाईट्रेशन रिएक्शन) के कारण, दिल्ली शहर के भीतर ओजोन सांद्रता कम होती है, और ५६-९८ माइक्रोग्राम प्रति घन मीटर (औसत ७६) के बीच पायी गयी है। ओजोन बनने की दो स्थितियों (एनओएक्स या वीओसी संवेदनशील स्थिति) होती है। इनके आधार पर, वर्ष २०१२ में ओजोन के स्रोत योगदानों का पता लगाने के लिए, आई.एस.ए.एम.- सी.एम.ए.क्यू. मॉडल का उपयोग किया गया। मासिक औसत आधार पर किए गए मूल्यांकन से पता चलता है कि एनसीआर के बाहर के क्षेत्रों का ओजोन सांद्रता में योगदान पूरे साल के दौरान प्रमुख है। ओजोन सांद्रता में एनसीआर के बाहर के क्षेत्रों की हिस्सेदारी पूरे एनसीआर, दिल्ली, और डाउनविंड क्षेत्र में क्रमशः ९२-९३%, ८८-९२% और ८७-८९% है। हालांकि, जब प्रति घंटा पैमाने पर इसका विश्लेषण किया गया, तो स्थानीय स्रोतों का हिस्सा महत्वपूर्ण पाया गया है। दिल्ली में प्रति घंटा ओजोन सांद्रता में स्थानीय स्रोतों का अधिकतम योगदान गर्मियों में ४६% तक और सर्दियों में २६% तक हो जाता है। इन स्थानीय स्रोतों में, प्रमुख योगदानकर्ता परिवहन (१३-३१%), बिजली उत्पादन (२-१०%), और गैर-ऊर्जा स्रोत (१-३%) हैं। दिल्ली शहर के डाउनवाइंड क्षेत्र, स्थानीय स्रोतों के उच्च योगदान को दिखाते हैं, जो मानसून के बाद के मौसम में ५६% तक पहुंच जाता है। यह ओजोन के दिल्ली से

नीचे के क्षेत्रों की ओर वायुमंडलीय परिवहन के कारण होता है। यह निष्कर्ष निकाला गया है कि जबकि एनसीआर में क्षेत्रीय योगदान काफी अधिक हैं, परंतु उच्च फोटो- रासायनिक गतिविधि के दौरान, स्थानीय स्रोत के योगदान बहुत महत्वपूर्ण हो जाते हैं।

निर्णायक रूप से, स्थानीय और साथ ही क्षेत्रीय योगदानकर्ताओं के लिए नियंत्रण उपायों की आवश्यकता है। ओजोन बनने की दो स्थितियों की तुलना में, नाकॅस -सीमित स्थिति का योगदान गर्मियों के महीनों में अधिक पाया जाता है। इसका मुख्य कारण गर्मियों के महीनों में निम्न नाकॅस / वीओसी अनुपात होता है। सर्दियों में, बायोजेनिक वीओसी उत्सर्जन कम, और नाकॅस / वीओसी अनुपात उच्च होता है, जो कि वीओसी -सीमित स्थिति को विकसित करता है। दिल्ली में बनी ओजोन में वीओसी -सीमित स्थिति का हिस्सा जून में १२% से बढ़कर दिसंबर में ५५% हो जाता है। यह गर्मियों से सर्दियों के मौसम में, नाकॅस से वीओसी सीमित स्थिति का परिवर्तन दर्शाता है।

एनसीआर के बाहर के क्षेत्रों की हिस्सेदारी छोड़कर, दिल्ली के डाउनवाइंड क्षेत्रों में, नाकॅस- सीमित स्थिति में, परिवहन का योगदान ४९-६५% है। बिजली उत्पादन का योगदान १२-२१% है। वीओसी सीमित स्थिति में परिवहन क्षेत्र का योगदान ३९-६६% तक, तथा बाष्पीकरणीय स्रोतों से ७-२२% तक होता है। कुछ महीनों में, ३४% तक योगदान खुले कृषि अवशेषों के जलने से भी होता है। दिल्ली के डाउनवाइंड क्षेत्रों में ओजोन में वीओसी सीमित स्थिति का हिस्सा जून में १४% से बढ़कर दिसंबर में ६५% हो जाता है।

भारत के शहरों में ओजोन सांद्रता का अनुमान लगाने के लिए यह अध्ययन सफलतापूर्वक फोटो-कैमिकल ट्रांसपोर्ट मॉडल के उपयोग को दर्शाता है। अध्ययन में दिल्ली-एनसीआर में ओजोन के स्रोतों और पूर्ववर्ती प्रदूषकों के योगदान का भी पता चलता है, जिसका उपयोग ओजोन के नियंत्रण के लिए स्थानीय और क्षेत्रीय पैमाने पर परिदृश्य विकास और नीति विश्लेषण के लिए भी किया जा सकता है।

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List of Abbreviations

AAQFS	: Australian Air Quality Forecasting System
AOT40	: Accumulated Concentration Over a Threshold of 40 ppb
AQI	: Air Quality Index
AURAMS	: A Unified Regional Air-quality Modelling System
BAU	: Business as Usual scenario
BC	: Boundary Conditions
BCON	: Boundary conditions contributions
BNMBF	: Normalized mean bias factor
ENMAEF	: Normalized mean absolute error factor
BS	: Bharat Stage
CAAQM	: Continuous Ambient Air Quality Monitoring Program
CAMx	: Comprehensive Air Quality Model with extensions
CBM	: Carbon Bond Mechanism
CCTM	: CMAQ Chemical Transport Model
CGRER	: Center of Global and Regional Environmental Research
CH ₄	: Methane
CMAQ	: Community Multi-scale Air Quality model
CNG	: Compressed Natural Gas
CO	: Carbon Monoxide
CO ₂	: Carbon Dioxide
CPCB	: Central Pollution Control Board
CSTR	: Completely stirred tank reactor
CTCZ	: Continental tropical convergence zone
‘d’	: Index of agreement
DCE	: Delhi college of Engineering, New Delhi
DG	: Diesel generator
DPCC	: Delhi Pollution Control Committee
EC	: Elemental Carbon
EF	: Emission Factor
EMEP	: European Monitoring and Evaluation Programme
EPA	: Environment Protection Agency
EURAD	: European Air Pollution Dispersion Model

G.NOIDA	: Greater NOIDA (New Okhla Industrial Development Authority)
GAINS	: Greenhouse Gas - Air Pollution Interactions and Synergies
GAW	: Global Atmosphere Watch programme
GEOS-Chem	: Goddard Earth Observing System (GEOS) chemical transport model
GRS	: Generic Reaction Set
GLO	: Ground Level Ozone
HDV	: Heavy duty vehicles
HF	: Hybrid forecast
H ₂ O ₂	: Hydrogen peroxide
HNO ₃	: Nitric Acid
HRVOC	: Highly Reactive Volatile Organic Compounds
ICAMS	: Integrated Climate and Air Quality Modelling System
ICON	: Initial conditions contributions
IMD	: Indian Meteorological Department
IoA	: Index of agreement
IGI	: Indira Gandhi International airport (IGI) airport
IPCC	: Intergovernmental Panel on Climate Change
ISAM	: Integrated Source Apportionment Module
ISCST3	: Industrial Source Complex short term model
ITO	: Income Tax Office (a traffic location in Delhi)
kg	: Kilogram
kt	: Kilotons
kt/yr	: Kilotons/year
kwh	: Kilowatt hour
LIRAQ	: Livermore Region Air Quality Models
LOTOS	: Long Term Ozone Simulation
LPG	: Liquefied Petroleum Gas
MAQSIP	: Multiscale Air Quality Simulation Platform
MATCH	: Multiscale atmospheric transport and chemistry model
MB	: Mean bias
MCIP	: Meteorology-Chemistry Interface Processor
ME	: Mean error
MLE	: Maximum likelihood
MM5	: Mesoscale Meteorological Model
MMSCMD	: Million standard cubic metre per day

MoM	: Method of moments
MOZART	: Model for OZone and Related Chemical Tracers
MS	: Mean subtraction
MSE	: Method of least squared error
MSSP	: Model system for soluble particles
MW	: Megawatt
NAAQS	: National Ambient Air Quality Standards
NAM	: North American Mesoscale Forecast System
NAMP	: National Air Monitoring Program
NAQFC	: National Air Quality Forecasting Capability
NCAR	: National Centre for Atmospheric Research
NCEP	: National Centres for Environmental Prediction
NCR	: National Capital Region
NH	: National Highway
NMB	: Normalized mean bias
NME	: Normalized mean error
NMOC	: Non-methane organic compound
NMSE	: Normalised Mean Square Error
NMVOC	: Non-Methane Volatile Organic Compounds
NO _x	: Nitrogen Dioxide
NO	: Nitric oxide
NO ₂	: Nitrogen dioxide
N ₂ O	: Nitrous oxide
NOIDA	: New Okhla Industrial Development Authority
NSSO	: National Sample Survey Organization
O ₃	: Ozone
Obs	: Observations
OC	: Organic Carbon
OSAT	: Ozone Source Apportionment Technology
OZIPR	: Ozone Isopleths Plotting Research
PATH	: Pollutants in the Atmosphere and their Transport over Hongkong
ppb	: Parts per billion
ppt	: Parts per trillion
PM	: Particulate matter
PM ₁₀	: Particulate matter less than 10 mm size

PM _{2.5}	: Particulate matter less than 2.5 mm size
r ²	: Coefficient of correlation
RADM	: Regional Acid Deposition Model
RA	: Ratio adjustment
RAQM	: Regional air quality model
RCG	: REM CALGRID model
RMSE	: Root Mean Square Error
ROM	: Regional Oxidant Model
RH	: Relative Humidity
RSPM	: Respirable Suspended particulate matter
RTM	: Regional Transport Model
SAPRC	: State-wide Air Pollution Research Centre
SL	: Silt Loading
SMRAQ	: Seasonal Model for Regional Air Quality
SO ₂	: Sulphur Dioxide
SPM	: Suspended particulate matter
STE	: Stratosphere–troposphere exchange
STEM	: Sulfur transport Eulerian model
TERI	: The Energy and Resource Institute
Tg	: Teragram
UAM	: Urban Airshed Model
UK	: United Kingdom
URM	: Urban-to-Regional Multiscale Airshed air quality model
US	: United States
USEPA	: United State Environment Protection Agency
USGS	: United States Geological Survey
UV	: Ultra Violet
VKT	: Vehicle Killometre Travelled
VOC	: Volatile organic Compounds
WHO	: World Health Organization
WMO	: World Meteorological Organization
WPS	: WRF Pre-processing system
WRF	: Weather Research Forecasting model