Developing Ozone Control Strategies in a “One-Atmosphere” Setting

An ORC Perspective

Panos G. Georgopoulos, Sastry S. Isukapalli, Shan He, Paul J. Lioy
and the ORC Team

presented at the Clean Air Council Meeting, March 9, 2011

Computational Chemodynamics Laboratory
Environmental and Occupational Health Sciences Institute (EOHSI)
170 Frelinghuysen Road, Piscataway, NJ 08854
The Ozone Research Center at EOHSI was established in 1989 with base funding from the NJDEP

• To provide scientific and technical support of regulatory studies

• To pursue research on the causes, mechanisms, dynamics and health effects of photochemical air pollution
  – enhancing the fundamental scientific understanding of photochemical air pollution systems and associated human exposures and health effects
  – providing the necessary scientific rationale for developing and implementing efficient air quality management strategies
    • with special focus on issues affecting the Northeastern United States and in particular the State of New Jersey

In the past 20 years the ORC evolved, gaining national recognition in the integrative study of air and multimedia pollution exposures and effects.

Related research centers and projects have been funded by NIH, USEPA, USDOE, USDOD, FAA, NJDHSS, ACC, and other agencies and organizations.
Acknowledgements

• The CCL Team
  – Panos G. Georgopoulos
  – Sastry Isukapalli
  – Chris Brinkerhoff
  – Sagnik Mazumdar
  – Jocelyn Alexander
  – Kristin Borbely
  – Teresa Boutillette
  – Linda Everett
  – Zhong-Yuan "Wheat" Mi
  – Christos Efstathiou *
  – Dwaipayan Mukherjee
  – Alan Sasso *
  – Pamela Shade
  – Spyros Stamatelos *
  – Xiaogang Tang
  – Yong Zhang
  – Peter Koutsoupias

*PhD awarded 2009-10

• NJDEP Personnel
  – Shan He
  – Linda Bonanno
  – Chris Salmi
  – Charles Pietarinen
  – Sharon Davis
  – Ray Papalski
  – Bill O’Sullivan
  – Tonalee Key
  – and many others....

• EOHSI/Rutgers Collaborators
  – Clifford Weisel
  – Tina Fan
  – Rob Laumbach
  – Charles Weschler
  – Leonard Bielory
  – Alan Robock
  – and many others....

• NYSDEC Collaborators
  – Christian Hogrefe
  – Gopal Sistla
  – Eric Zalewsky
Understanding health (and ecological) effects and developing rational/optimal control strategies is complicated by the fact that air pollution is a multiscale problem in terms of both the environmental and the biological processes involved.
ORC/CCL employs a “One-Atmosphere” approach to account for physical/chemical transformations (e.g. involving ·OH) over multiple spatial/temporal scales that “couple” the dynamics of multiple gaseous and particulate air pollutants.
For most people the majority of exposures to airborne contaminants takes place through contact and inhalation of chemicals in indoor (residential or occupational) microenvironments. The air in these microenvironments contains a complex mixture of contaminants including those entrained from outdoor (ambient) air, those emitted indoors, and those formed via chemical transformations in indoor air (e.g. ultrafine particles formed from the interaction of entrained ozone with emissions from household air fresheners and solvents).
Often the most significant exposures to airborne contaminants take place in confined (residential and public) microenvironments.

For most people, the majority of exposures to airborne contaminants take place through contact and inhalation of chemicals in indoor (residential or occupational) microenvironments. The air in these microenvironments contains a complex mixture of contaminants including those entrained from outdoor (ambient) air, those emitted indoors, and those formed via chemical transformations in indoor air (e.g., ultrafine particles formed from the interaction of entrained ozone with emissions from household air fresheners and solvents).
Ozone levels and reaction by-products in aircraft cabins

C2 in-flight ozone concentration
westbound trans-continental
Q1 2009, B 757 – 200, No ozone converter

Sampling duration: 5.0 h
Max 1-minute ozone (ppb): 103
Max 1-hour ozone (ppb): 84
Sample avg. concentration (ppb): 54

Occupants
Skin oil (i.e., squalene, oleic acid, unsaturated sterols), isoprene, nitric oxide (NO),

Carpet & backing
4-PCH, 4-VCH, unsaturated fatty acids

Seats
Skin oil, fabric

Soiled air filters
Unsaturated organics associated with captured particles

Saturated aldehydes produced by ozone reactions

Formaldehyde, acetaldehyde, sum C4-C8, nonanal, decanal

Transatlantic flight ozone concentrations
B 747 - January 2009 with ozone converter

Data and slides provided by C. Weshler and C. Weisel
## National Ambient Air Quality Standards (NAAQS)

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>Primary Standards</th>
<th>Secondary Standards</th>
<th>Attainment Status</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Level</td>
<td>Date</td>
<td>Averaging Time</td>
</tr>
<tr>
<td><strong>CO</strong></td>
<td>9 ppm</td>
<td>1971</td>
<td>8-hour</td>
</tr>
<tr>
<td></td>
<td>35 ppm</td>
<td>1971</td>
<td>1-hour</td>
</tr>
<tr>
<td><strong>Lead</strong></td>
<td>1.5 μg/m³</td>
<td>1978</td>
<td>Quarterly Average</td>
</tr>
<tr>
<td></td>
<td>0.15 μg/m³</td>
<td>2008</td>
<td>Rolling 3-Month Average</td>
</tr>
<tr>
<td><strong>NO₂</strong></td>
<td>53 ppb</td>
<td>1971</td>
<td>Annual</td>
</tr>
<tr>
<td></td>
<td>100 ppb</td>
<td>2010</td>
<td>1-hour</td>
</tr>
<tr>
<td><strong>PM₁₀</strong></td>
<td>150 μg/m³</td>
<td>1987</td>
<td>24-hour</td>
</tr>
<tr>
<td><strong>PM₂.₅</strong></td>
<td>15.0 μg/m³</td>
<td>1997</td>
<td>Annual</td>
</tr>
<tr>
<td></td>
<td>35 μg/m³</td>
<td>2006</td>
<td>24-hour</td>
</tr>
<tr>
<td></td>
<td>12.0 μg/m³?</td>
<td>?</td>
<td>Annual</td>
</tr>
<tr>
<td></td>
<td>30 μg/m³?</td>
<td>?</td>
<td></td>
</tr>
<tr>
<td><strong>Ozone</strong></td>
<td>120 ppb</td>
<td>1979</td>
<td>1-hour</td>
</tr>
<tr>
<td></td>
<td>80 ppb</td>
<td>1997</td>
<td>8-hour</td>
</tr>
<tr>
<td></td>
<td>75 ppb</td>
<td>2008</td>
<td>8-hour</td>
</tr>
<tr>
<td></td>
<td>60 – 70 ppb ?</td>
<td>?</td>
<td></td>
</tr>
<tr>
<td><strong>SO₂</strong></td>
<td>30 ppb</td>
<td>1971</td>
<td>Annual</td>
</tr>
<tr>
<td></td>
<td>140 ppb</td>
<td>1971</td>
<td>24-hour</td>
</tr>
<tr>
<td></td>
<td>75 ppb</td>
<td>2010</td>
<td>1-hour</td>
</tr>
</tbody>
</table>
Ambient air quality has been gradually but steadily improving in NJ: Overall trend for all criteria air pollutants in NJ, 1965-2009

Maximum Pollutant Concentrations in New Jersey, 1965-2009
(Source: EPA AirData)

Percentage of ambient criteria pollutant levels above or below the corresponding National Ambient Air Quality Standard (NAAQS)
Ambient air quality has been gradually but steadily improving in NJ:

Monitored concentrations of (a) benzene (1990-2007) and (b) formaldehyde (1996-2007) in NJ

... and this is taking place in spite of the increase in factors that could result in higher emission levels, such as vehicle miles traveled per person in NJ.

However, despite the progress, very substantial challenges remain (especially with the ambient standards becoming more stringent): Counties violating the March 2008 ozone standard of 0.075 ppm

(Based on 2006 – 2008 Air Quality Data)

322 of 675¹ monitored counties violate the standard

Notes:
1. Counties with at least one monitor with complete data for 2006 – 2008
2. To determine compliance with the March 2008 ozone standards, the 3-year average is truncated to three decimal places.
Nonattainment area designations for the 2006 24-hour fine particle (PM2.5) standards

EPA Designation
- Attainment/Unclassifiable
- Nonattainment - Whole County
- Nonattainment - Partial County

[Map showing areas designated as attainment or nonattainment for PM2.5 standards]
Developing ambient ozone control strategies to meet the new standards: Screening runs performed by the OTC – ongoing work

- To investigate the level of emissions reductions needed to achieve the current NAAQS of 75 ppb and the potentially lower new NAAQS in the 60 to 70 ppb range

- Approach
  - Screening simulations applying across-the-board reduction in emissions, as well as a simulation approximating OTC-recommended national and local measures
  - 2007 meteorology replicated by WRF for April 1 – October 31 (base case)
  - Anthropogenic “proxy” emissions
    - Actual 2007 for point and non-road sources within MANE-VU; other point sources from EPA CHIEF 2005; remaining source sector emissions were interpolated from 2002 and 2009 inventories from 2002 SIP
    - Biogenic 2007 emissions based on MEGAN
    - Photochemical model – CMAQv4.7 with CB5 chemistry
    - Modeling domain: 12 km Eastern US; boundary conditions kept at “clean” background levels

- Participants in this effort:
  - NJDEP/ORC; UMD/MDE; NYSDEC; MARAMA; OTC
## OTC States and modeling domain

### NOx Emissions (tons/yr)
- **EGU Point**: 1,818,914
- **Biogenic Area**: 114,670
- **Area**: 1,894,211
- **Nonroad Mobile**: 2,892,301
- **Nonroad Point**: 1,818,914
- **Mobile**: 5,041,231

### VOC emissions (tons/yr)
- **Mobile Point**: 1,151,217
- **Mobile**: 1,939,410
- **Nonroad**: 2,259,879
- **Area**: 5,501,846
- **Biogenic**: 23,263,840
- **Non-EGU Point**: 1,818,914

---

**OTC States**

- 36 km domain
- 12 km domain
Distribution of domain VOC emissions

- Anthropogenic VOC emissions are dominant in urban areas
- Biogenic VOC emissions are dominant in forested areas, especially in the south
# Base case model performance

August 2, 2007

August 3, 2007

<table>
<thead>
<tr>
<th>Region</th>
<th>Data Pairs</th>
<th>Mean Observed</th>
<th>Mean Model</th>
<th>Mean Bias (ppb)</th>
<th>Mean Error (ppb)</th>
<th>Normalized Mean Bias (Percent)</th>
<th>Normalized Mean Error (Percent)</th>
<th>Root Mean Square Error (ppb)</th>
<th>Correlation Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain-wide</td>
<td>115,712</td>
<td>49.7</td>
<td>51.9</td>
<td>2.2</td>
<td>9.5</td>
<td>4.4</td>
<td>19.2</td>
<td>12.4</td>
<td>0.7</td>
</tr>
</tbody>
</table>
OTC screening control scenarios

- “Scenario 3” includes MOVES adjustments to MOBILE6 emissions
- approximates an overall 55% NOx reduction domain-wide:
  - Point: 65% reduction (includes reductions from ICI boilers and cement kilns and a 900,000 ton regional trading cap on EGUs)
  - On-road: 75% reduction (approximates a 2020 national LEV 3)
  - Non-road: 35% reduction (includes reductions from marine and locomotive engines)
  - NOx in OTR States: additional 5% reduction across all sectors in the OTR
Relative ozone reductions: Simulations for June 1 – August 31, 2007

- Ozone reductions from “Scenario 3” run fall between those from the across-the-board reduction simulations
- NO$_x$ focused emission reductions show less benefit for urban core areas
• In N50/V30 across-the-board reductions, hot spots remain in urban areas
• Hot spots are further reduced in “Scenario 3” and N70/V30 reduction scenarios
Comments regarding the screening simulations

• Caveats
  – Use of proxy emissions through interpolated inventories
  – Simplified “MOVES-like” adjustment to MOBILE6 emissions not fully tested
  – Use of “time invariant clean” boundary conditions
  – Simplified across-the-board emission reduction approaches

• Preliminary conclusions
  – 2007 episode meteorology and ozone patterns have been qualitatively captured
  – Ozone levels are overestimated during episodes over the OTC states - possible cause is the “MOVES-like” component
  – In general the N70/V30 reduction case provides increased response of 7 to 11 ppb over N50/V30
  – All screening simulations generally give lower ozone reductions in core urban areas such as Bayonne, NJ and Bronx, NY
  – A 50% across the board NOx reduction does not achieve full attainment, particularly for the I-95 corridor; a 70% reduction appears to get most areas of the OTR into the low range (60-65 ppb) of the proposed ozone NAAQS
  – “Scenario 3” (approximately a 55% reduction) brings several areas of the OTR into the middle of the proposed range

• Ongoing and future activities
  – Model evaluation and coordination among centers; use of updated inventories; use of dynamic boundary conditions (from Georgia DEP); future year simulation
Selected examples from relevant ongoing research projects

• Impact of uncertainties in biogenic emissions on effectiveness of pollution control strategies
  Xiaogang Tang, Christian Hogrefe, Shan He, Sastry Isukapalli, Panos Georgopoulos

• Modeling effects of climatic change on biogenic aeroallergens in a multi-pollutant framework
  Yong Zhang, Christos Efstathiou, Sastry Isukapalli, Leonard Bielory, Panos Georgopoulos

• GIS based planning and management support system for emergency events involving airborne releases from transportation incidents
  Sastry Isukapalli, Jocelyn Alexander, Chris Yung, Panos Georgopoulos

• Investigating localized exposures to airborne contaminants using computational fluid dynamics (CFD)
  Sagnik Mazumdar, Panos Georgopoulos, Sastry Isukapalli

• Modeling the uptake and biological effects of exposures to trichloroethylene using physiologically based toxicokinetic and toxicodynamic modeling
  Chris Brinkerhoff, Sastry Isukapalli, Dwaipayan Mukherjee, Panos Georgopoulos

• Modeling the atmospheric fate and inhalation dosimetry of nanoparticles
  Pam Shade, Alan Sasso, Sastry Isukapalli, Panos Georgopoulos

• A modeling framework for assessing risk from engineered nanoparticles in the environment
  Alan Sasso, Pam Shade, Chris Brinkerhoff, Sastry Isukapalli, Panos Georgopoulos

• An exposure information system for studying effects of air quality on birth outcomes and child development (part of the National Children’s Study)
  Chris Brinkerhoff, Sastry Isukapalli, Paul Lioy, Panos Georgopoulos
Impact of uncertainties in biogenic emissions on predicted ozone and PM2.5 levels: effect on development of control strategies

• CMAQ simulations driven with outputs from MEGAN and BEIS emissions modeling systems
• Control scenario with 40% across the board anthropogenic NOx reductions for year 2012
• Impact on ozone (approximately 5%) and PM$_{2.5}$ levels (1-2%)
• Indirect impact on inorganic PM$_{2.5}$

Relative Reduction Factors (RRF) for Ozone

RRF difference (MEGAN – BEIS) for PM$_{2.5}$ OM (left) and sulfate PM (right)
Modeling effects of climatic change on biogenic aeroallergens in a multipollutant framework

Vegetation database in the Biogenic Emissions and Landuse Database (BELD3)

Modeled concentrations using CMAQ-pollen: snapshot at 4 pm on April 16, 2002

Representative future meteorology:
Seasonal average change in temperature and precipitation estimated by the CCSM driving AOGCM and MM5I

[Source: NARCCAP]

CCSM: Community Climate System Model
AOGCM: Atmospheric and Oceanic General Circulation Model
MM5I: MM5 - PSU/NCAR mesoscale model
NARCCAP: North American Regional Climate Change Assessment Program (http://www.narccap.ucar.edu/)
GIS based planning and management support system for emergency events involving transportation incidents

Real Time/On Line

Other Lab & Field Data

MET & GIS (TOPO, RECEPTOR) DATA

Controlled Experiments & Research Monitoring Network

Real Time Sensor & Monitor Data

e.g. RAMS/HYPACT FLUENT linked with MENTOR (CCL-EOHSI)

Evaluation of Assumptions

Systematic Simplification

Real Time Assimilation

Guidance & Decision Support

Controlled Experiments & Research Monitoring Network

SOURCE & CONTAMINANT DATA

Regional Atmospheric Modeling System/Hybrid Particle And Concentration Transport Model (RAMS/HYPACT)

Hazard Prediction and Assessment Capability (HPAC) - Defense Threat Reduction Agency (DTRA)

GIS based planning and management support system for emergency events involving transportation incidents

Real Time

Real Time/On Line

Off-Line Scenario Based

Trained EM Personnel

Center Scientists

Research Scientists

Model Application & Operators
Investigating localized exposures in confined public spaces using computational fluid dynamics (CFD)

Experimental facility
Kansas State University

CFD model

CFD mesh

Pesticide deposition rate

Experiments vs CFD

Lap

Seat top

Pesticide deposition rate (µg/cm²-s): 1E-05  5E-05  0.0001  0.0005  0.001  0.005
Investigating localized exposures using microscale modeling: neighborhood-scale analysis in an urban environment

Transportation incident involving chlorine release (small truck)

Case 1: Continuous release (1 ton/h)
Case 2: Instantaneous release (1 ton)
Wind Speed: 2 m/s

Iso-contours of 20 mg/m³ [AEGL-3; possible fatalities; severe effects; medical attention]
Simulated using QUIC (Quick Urban & Industrial Complex) Dispersion Modeling System: developed by Los Alamos National Laboratory (http://www.lanl.gov/projects/quic/)
Modeling the atmospheric fate and inhalation/whole body dosimetry of fine and ultrafine particles

MENTOR time course model estimates and confidence intervals for total radioactivity measured in blood, along with corresponding experimental data following exposure to carbon nanoparticles labeled with 99m-technetium. Assumptions based on the study by Pery, et al. (2009), and data used for evaluation are from Nemmar, et al. (2002).

Evaluation of respiratory fine and ultrafine (nano-) particle deposition predictions from MPPD2, ICRP, and MENTOR models with experimental data were taken from Chalupa et al. (2004) and Daigle et al. (2003).
A modeling framework for assessing risk from nanoparticles in the environment
An exposure information system for studying effects of air quality on birth outcomes and child development (part of the NCS effort)

Premature, low weight, and very low weight births and PM$_{2.5}$ levels for 2008 in the U.S.

Premature, low weight, and very low weight births and median household income for 2008 in the U.S.
Acknowledgments: Current research projects relevant to the ORC mission

- **NJ DEP**
  - Base funding for the Ozone Research Center (ORC) at EOHSI

- **NJ DHSS**
  - HIPPOCRATES – Mobile Access

- **NIH**
  - Center for Environmental Exposure and Disease (CEED) at EOHSI
  - National Children’s Study (NCS)
  - Respiratory Effects of Silver and Carbon Nanomaterials (RESAC)

- **USEPA**
  - Base support for the Center for Exposure and Risk Modeling (CERM) and for the Environmental Bioinformatics and Computational Toxicology Center (ebCTC)
  - Risk Assessment for Manufactured Nanoparticles Used in Consumer Products (RAMNUC)
  - Climatic Change and Allergic Airway Disease (CCAAD)

- **USDOD**
  - University Center for Disaster Preparedness and Emergency (UCDPER)

- **FAA**
  - Development of Risk Paradigm for Pesticides and Ozone/Ozone By-Products
Concluding Comments

- ORC is committed to supporting regulatory needs of the State of NJ and related NJDEP activities

- A range of modeling and analysis tools have been developed at ORC/CCL and are being applied not only to ozone, but also to inhalation (and total) exposures involving PM, air toxics, bioaerosols, nanoparticles, and multimedia contaminants (pesticides, solvents, heavy metals, etc.) in the ambient and in confined environments and microenvironments
  
  - Multiple existing modeling tools have been applied and tested (MM5, RAMS, HYPACT, HYSPLIT, M3/CMAQ, CAMx, ASPEN, AERMOD, HPAC, FLUENT, CFX; etc.)
  
  - Databases have been (or are being) assembled and restructured so as to facilitate future analyses (statistical and GIS)
  
  - A comprehensive and extensible new modeling framework (MENTOR) has been designed and implemented collaboratively with USEPA and is being applied to various situations of direct relevance to NJ and the region

- The “One Atmosphere” is evolving into the “One Environment” model; “Person Oriented Modeling” is central in this approach
  
  - These concepts are slowly being “fused” into EPA regulatory tools and practices
  
  - ORC aims to keep working closely with NJDEP and other regional organizations to support current/future use of “best science” in regulatory practices