

Air Pollutants – The Old and the New

An overview of current studies at the Ozone Research Center

Panos G. Georgopoulos

Presented at the ORC Workshop
December 3, 2012

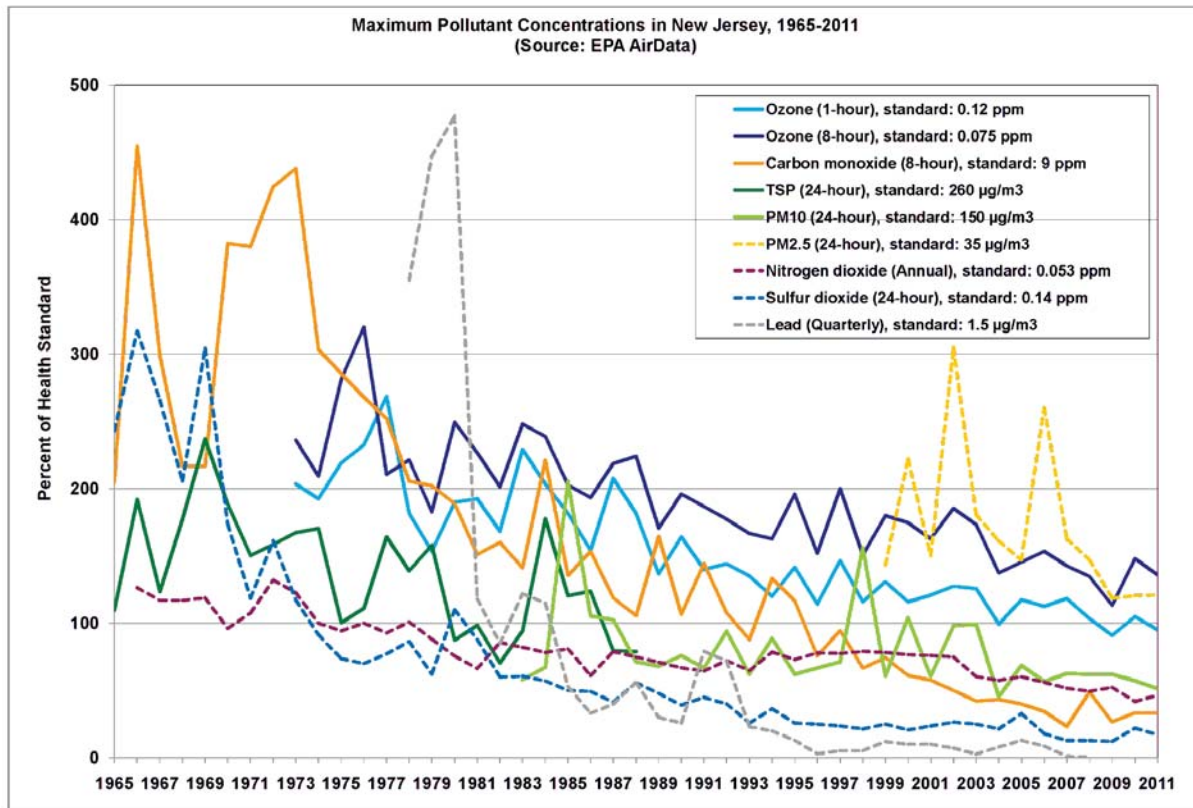
Computational Chemodynamics Laboratory
Environmental and Occupational Health Sciences Institute (EOHSI)
170 Frelinghuysen Road, Piscataway, NJ 08854



CCL Computational Chemodynamics Laboratory

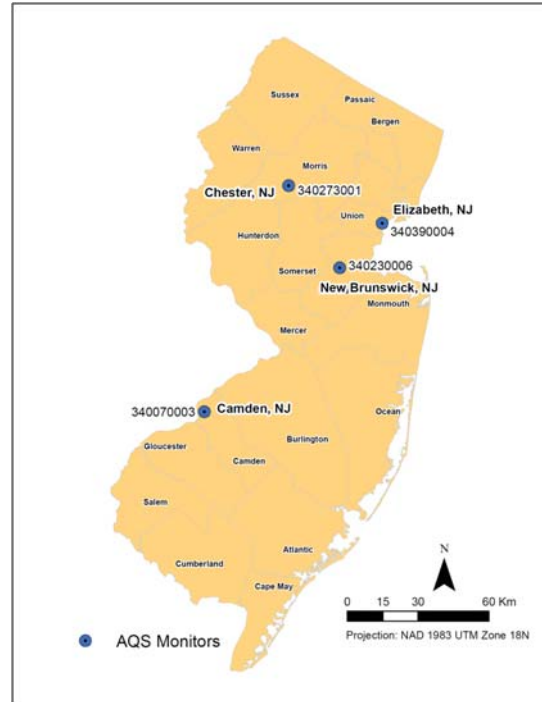
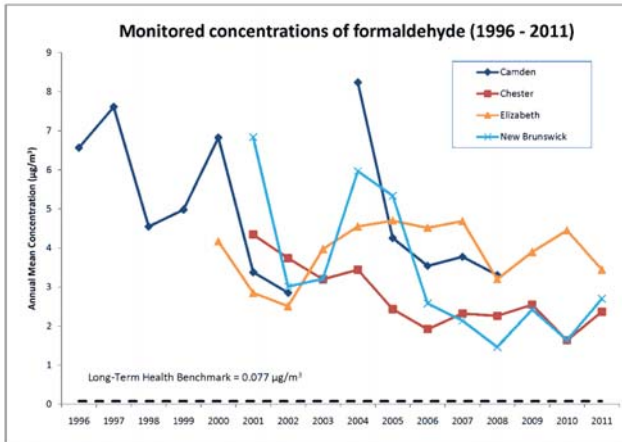
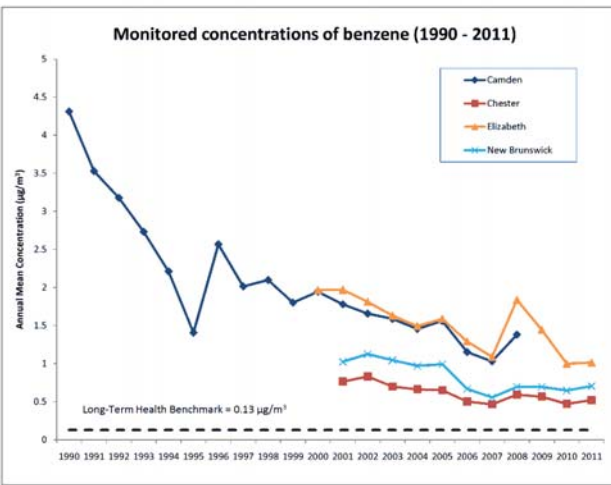


Ambient air quality has been gradually but steadily improving in NJ: Overall trend for all criteria air pollutants in NJ, 1965-2011

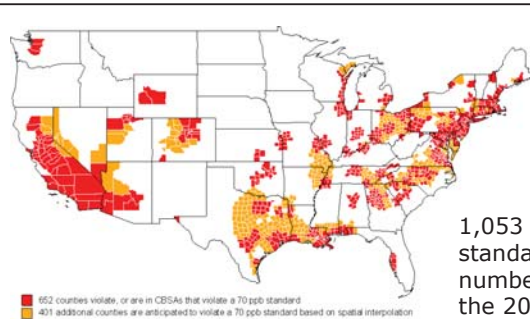


Percentage of ambient criteria pollutant levels above or below the corresponding National Ambient Air Quality Standard (NAAQS)

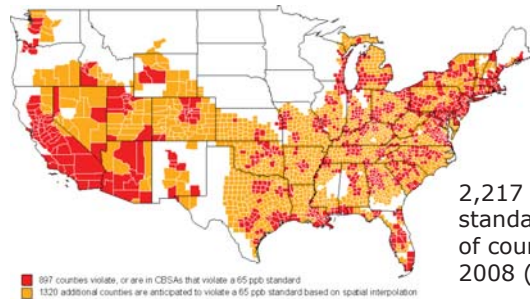
Ambient levels of monitored air toxics have also been gradually but steadily improving in NJ



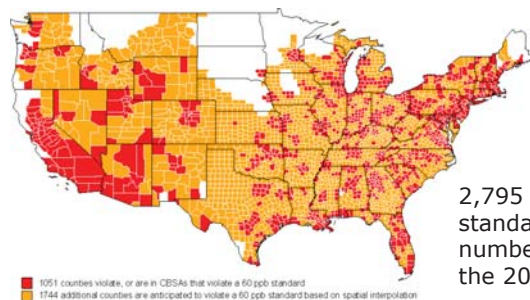
3



1,053 counties violate a 70 ppb standard (three times the number of counties that violate the 2008 (75 ppb) standard)



2,217 counties violate a 65 ppb standard (six times the number of counties that violate the 2008 (75 ppb) standard)



2,795 counties violate a 60 ppb standard (eight times the number of counties that violate the 2008 (75 ppb) standard)

Ozone compliance remains a major challenge, especially as new standards are considered

The National Association of Manufacturers (NAMS) has estimated substantial extent of standard violations, based on 2008-2010 monitor data, for more stringent forms of the standard

4

Mission and research approach of the Ozone Research Center

The original mission of the Ozone Research Center was to perform:

- Research to study the causes, dynamics and effects of photochemical air pollution (smog):
 - at the fundamental level
 - with special focus on issues and air quality problems affecting the Northeastern United States and in particular the State of New Jersey

Consistent with the original mission the ORC over the past 23 years has completed numerous projects related to:

- enhancing the 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

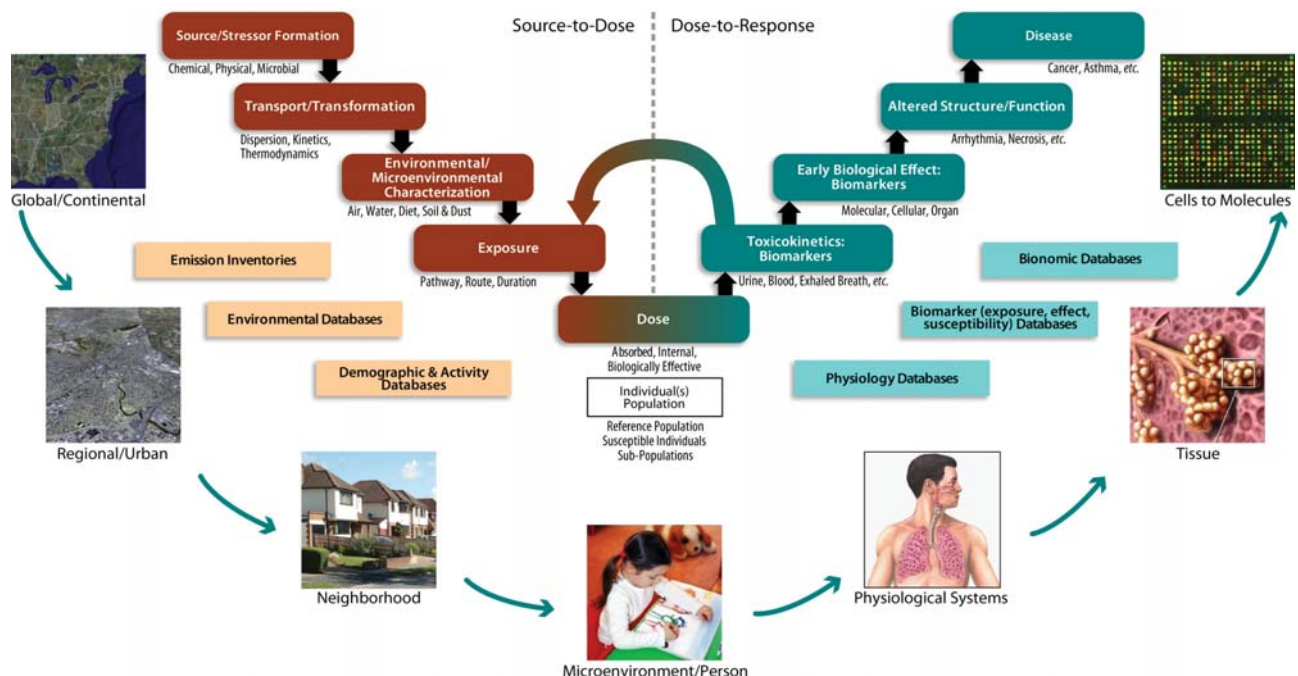
The **research approach** at ORC has been promoting the concepts of:

- **multiscale source-to-dose-to-effect modeling**
- **“one-atmosphere/one-environment” modeling**, accounting for environmental and biological interactions of co-occurring contaminants
- **“person-oriented” modeling**, accounting for behavior and exposure biology
- **life-cycle analysis** and spatiotemporal modeling

5

Air pollution is a multiscale problem
for both the environmental and the biological processes involved:

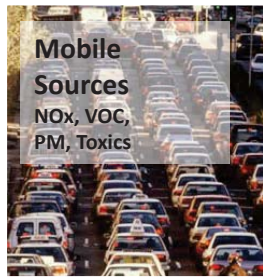
Treating it as such is critical for understanding its effects and for developing rational/optimal control strategies



From: Georgopoulos, et al. (2009). Environmental Manager (October): 26-35

6

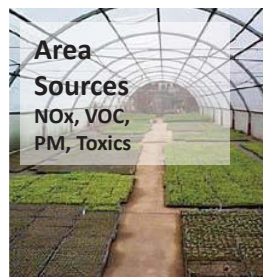
The "One-Atmosphere" concept provides consistency in environmental quality and health risk modeling and management



Cars, trucks, planes, boats, etc.



Power plants, refineries/chemical plants, etc.



Residential, farming, commercial, biogenic, etc.

Chemistry
Meteorology

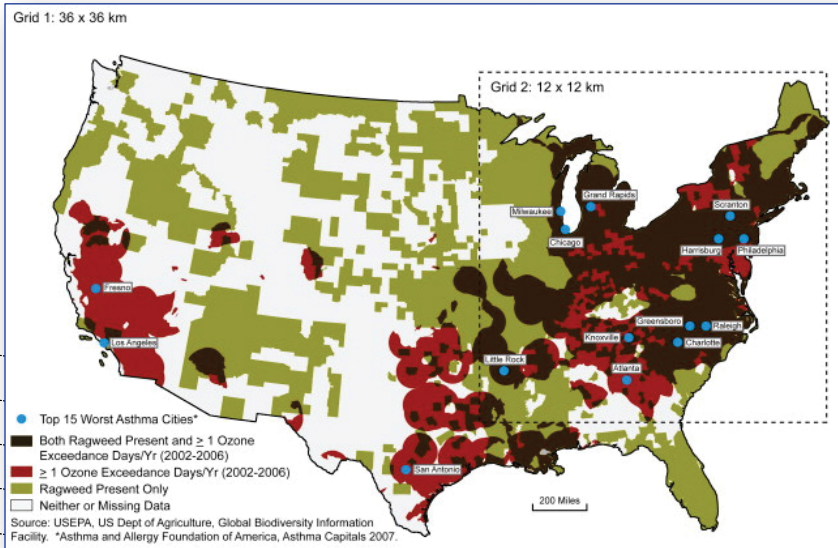
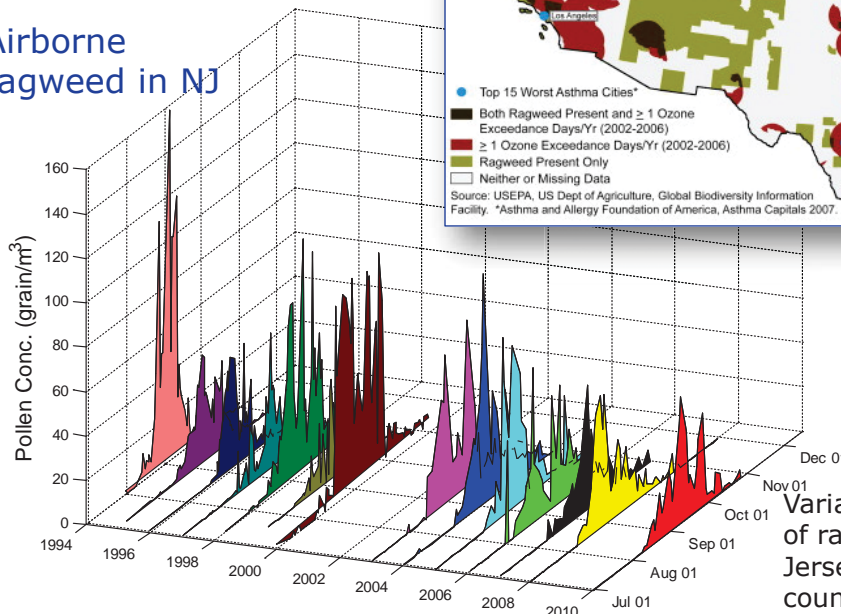
- Ozone
- PM
- Acid Rain
- Visibility
- Air Toxics
- Atmospheric Deposition
- Aeroallergens
- Climate Change



Slide adapted from EPA/OAQPS AQMG

Ozone and pollen are associated with asthma attacks and high levels of both co-occur in space and time especially in the NE US

Airborne ragweed in NJ



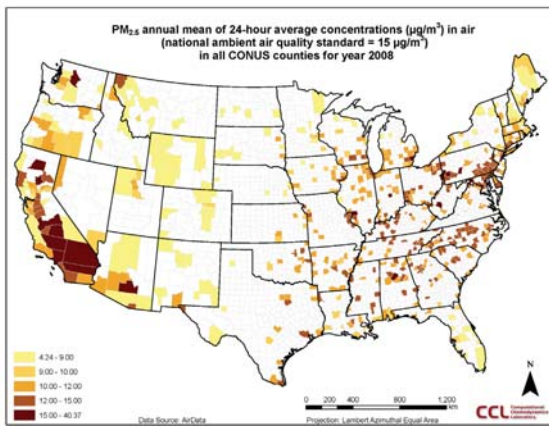
Variation of mean daily concentrations of ragweed pollen in Southern New Jersey: Data of daily airborne pollen count from the pollen monitoring stations in Cherry Hill, NJ

Selected examples from ongoing research projects

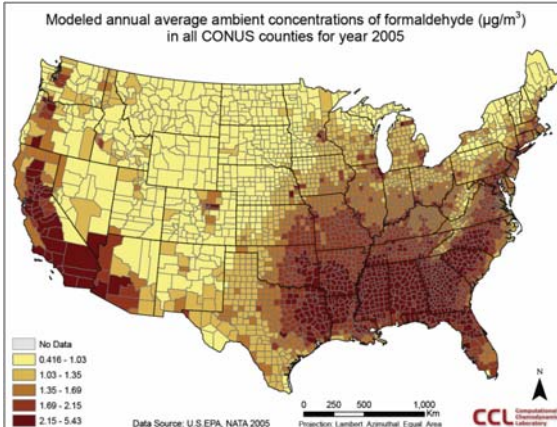
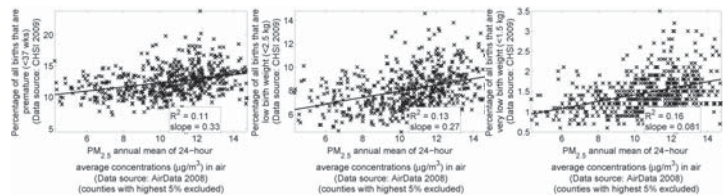
- Evaluating effectiveness of regional photochemical pollution control strategies***
 Xiaogang Tang, Christian Hogrefe, Michael Ku, Winston Hao, Eric Zalewsky, Kevin Civerolo, Jin-Sheng Lin, Shan He, Tonalee Key, Panos Georgopoulos
- Modeling effects of climatic change on biogenic aeroallergens***
 Yong Zhang, Leonard Bielory, Lai-yung Ruby Leung, Zhongyuan Mi, Panos Georgopoulos
- GIS-based management support system for emergency events**
 Paul Liroy, Michael Greenberg, Steven Royce, Jocelyn Alexander, Panos Georgopoulos
- Assessing risks from pesticide exposures in airline cabins during transatlantic flights**
 Yong Zhang, Panos Georgopoulos, Cliff Weisel
- A Tiered Exposure Ranking (TiER) system for studying effects of air quality and other factors on birth outcomes and child development and health***
 Panos Georgopoulos, Jocelyn Alexander, Shu Xu, Zhongyuan Mi, Steven Royce, Paul Liroy
- Characterizing residential and occupational exposures to WTC contaminants***
 Panos G. Georgopoulos, Zhongyuan Mi, Steven Royce, Jocelyn Alexander, Paul J. Liroy
- Development and testing of a system for Prioritization/Ranking of Toxic Exposures with GIS Extension (PRoTEGE), focusing on Contaminants of Emerging Concern (CEC)**
 Steven Royce, Dwaipayan Mukherjee, Zhongyuan Mi, Shu Xu, Panos G. Georgopoulos
 - Ongoing development of plans for merging PRoTEGE and DuPont's METIS (collaborators: John Gannon and Mario Chen)
- Multiscale modeling framework for assessing exposures, doses, and biological effects from "natural" and engineered nanoparticles******
 Dwaipayan Mukherjee, Steven Royce, Shu Xu, Pam Shade, Panos Georgopoulos

9

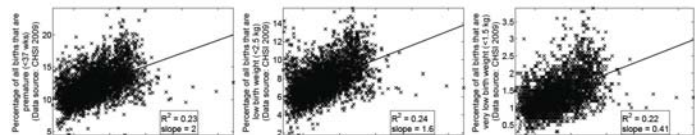
Example of One-Atmosphere modeling for inhalation exposures and risks: A tiered system for studying effects of air quality on birth outcomes and child development and health



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



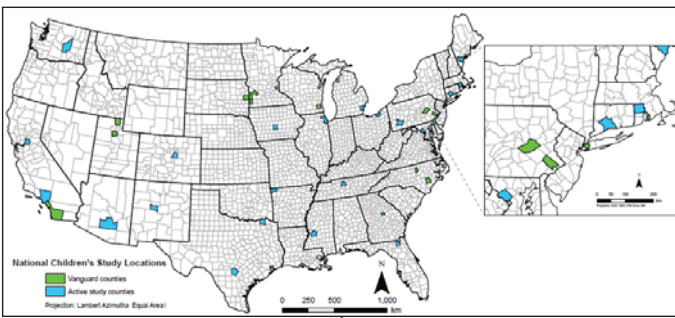
Premature, low weight, and very low weight births and modeled ambient formaldehyde levels for 2005 in the U.S.



10

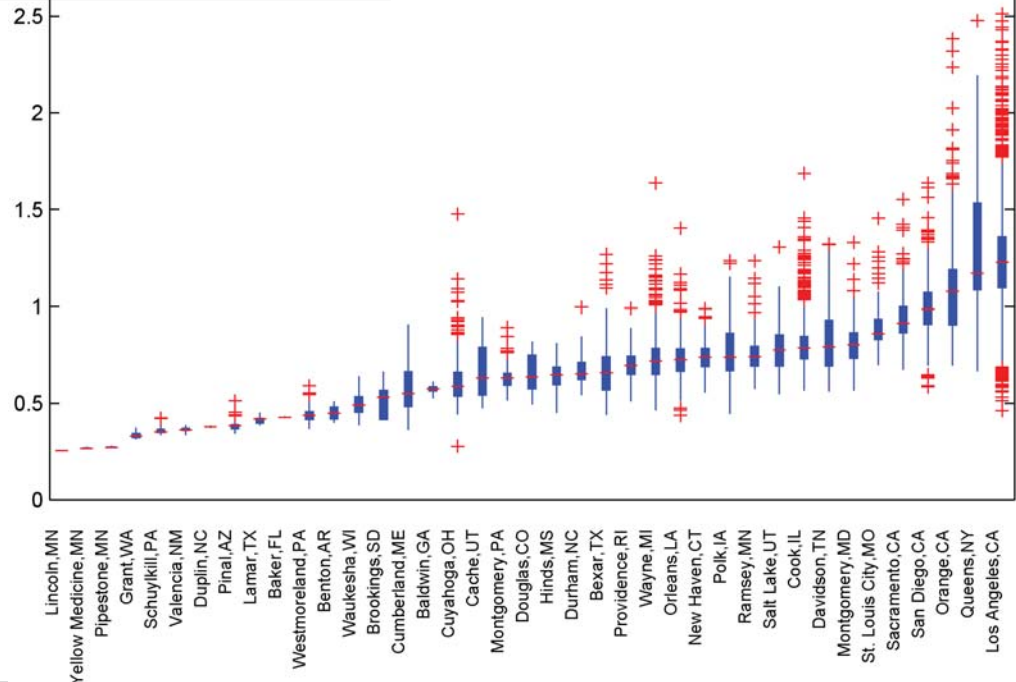
A health endpoint-specific* inhalation Exposure Index (EI) for the counties of the National Children's Study

*Premature birth hypothesizing
an inflammatory mechanism



40 active NCS counties

An endpoint-specific Inhalation Exposure Index was calculated for the "inflammatory" criteria pollutants (ozone, PM2.5, NO2, SO2) and 42 HAPs (air toxics) using observed and modeled airborne levels, weighted by reference concentrations relevant to inflammation or irritation



An example of Person-Oriented Modeling: Ranking occupational exposures of WTC responders and cleanup workers (9/2001-6/2002)

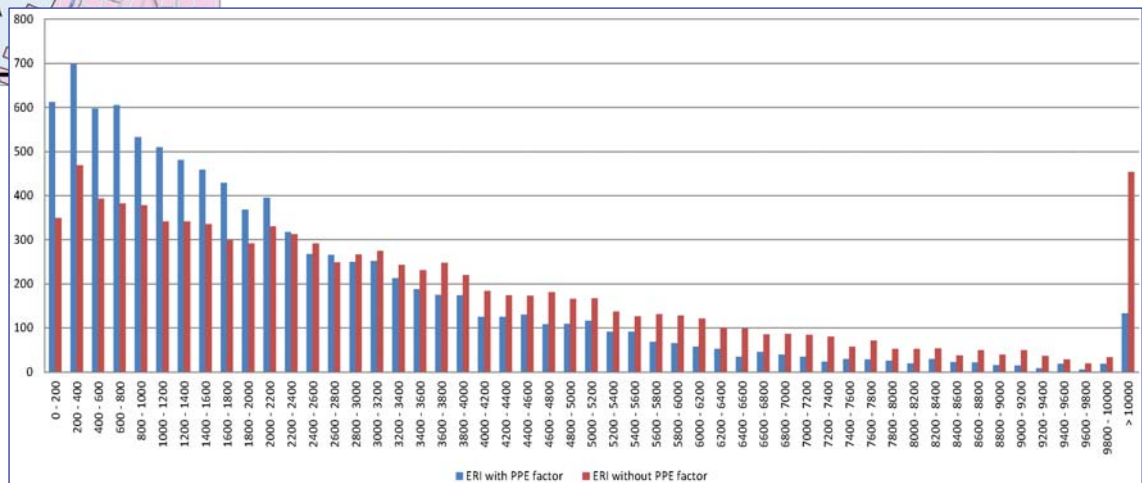
- A WTC "Exposure Ranking Index" (ERI) developed to characterize the relative rank of potential exposures of workers related to post-9/11 activities.

ERI involves factors related to

- type of activity,
- duration,
- location,
- time/date,
- Microenvironment,
- type and usage of personal protective equipment, etc., associated with each "exposure event" (such as a work shift)

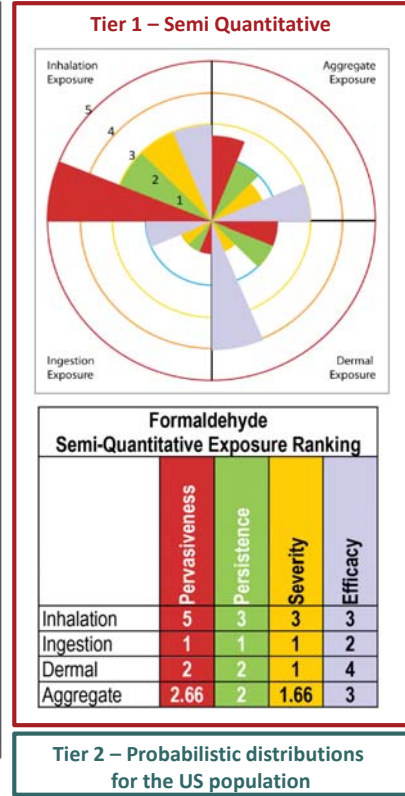
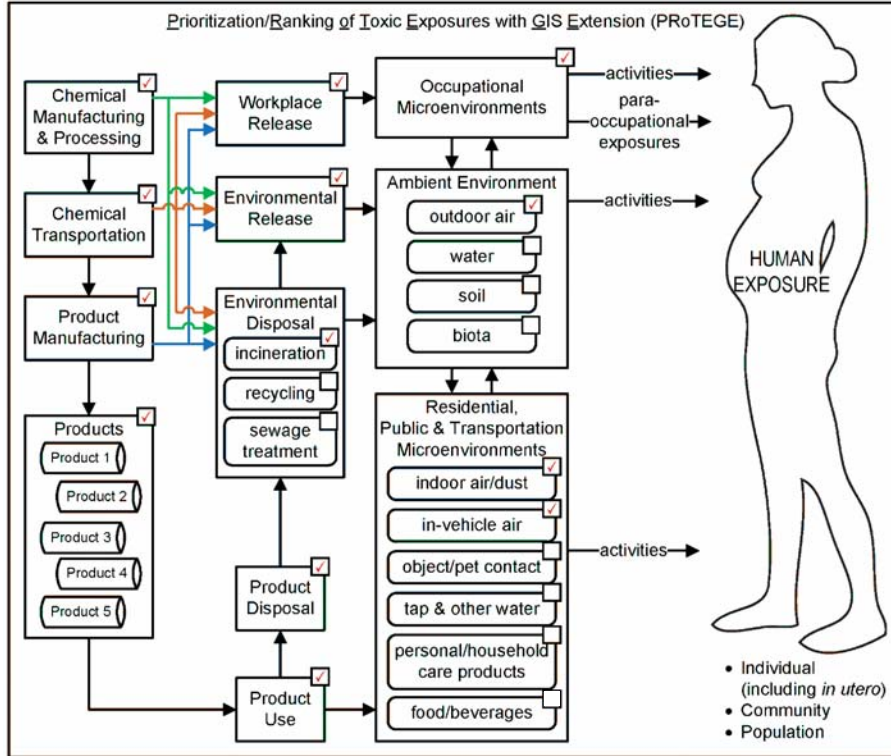


Cohort of 27,449 WTC responders: data maintained by the MSSM WTC Health Program Data Center (WTC-HPDC); Over 620 exposure-related fields per record



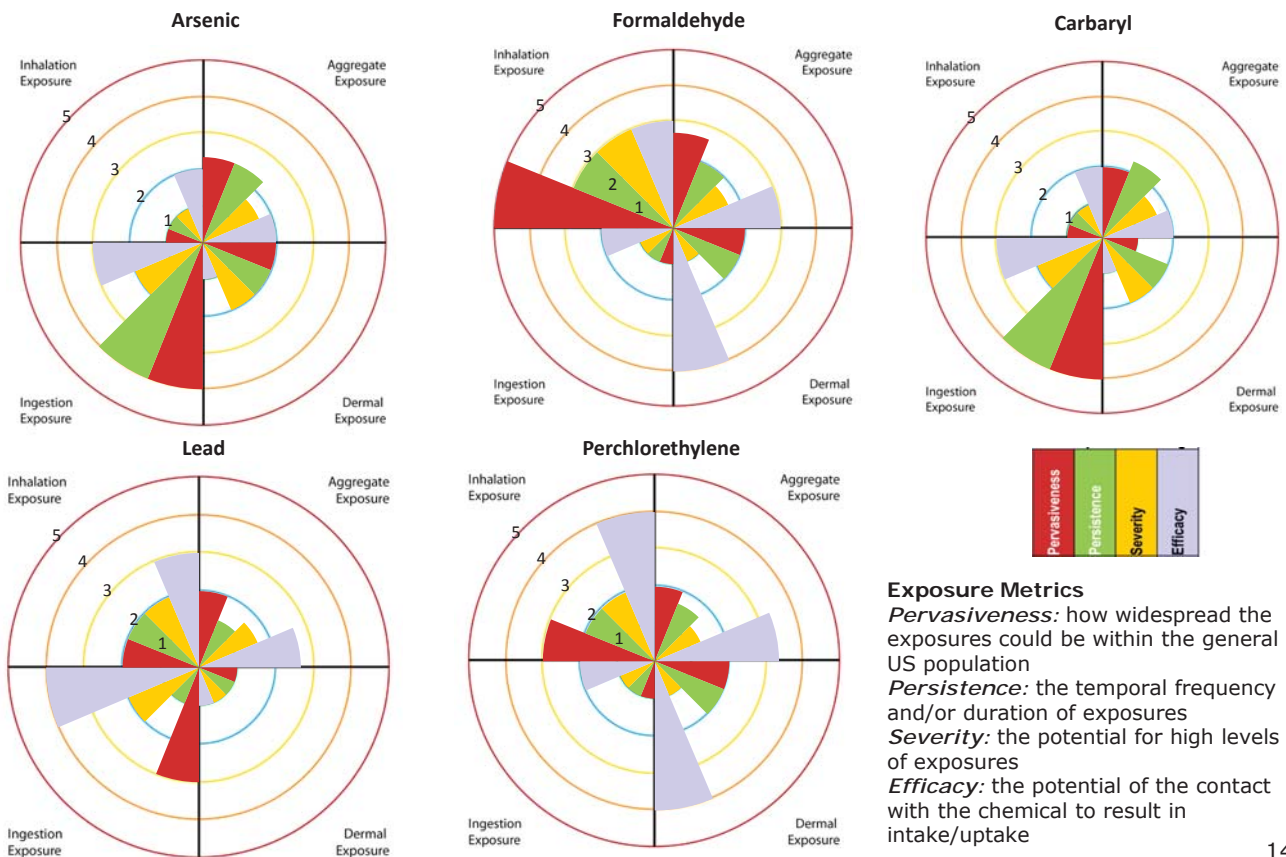
PRoTEGE - a tiered "Life-Cycle Analysis" modeling system that supports exposure-based prioritization and ranking of chemicals

PRoTEGE utilizes reduced components of the comprehensive MENTOR[†] system to provide a simplified modeling platform employing extant data and modules for the "screening" assessment of human exposures associated with toxics in various (micro)environments and products



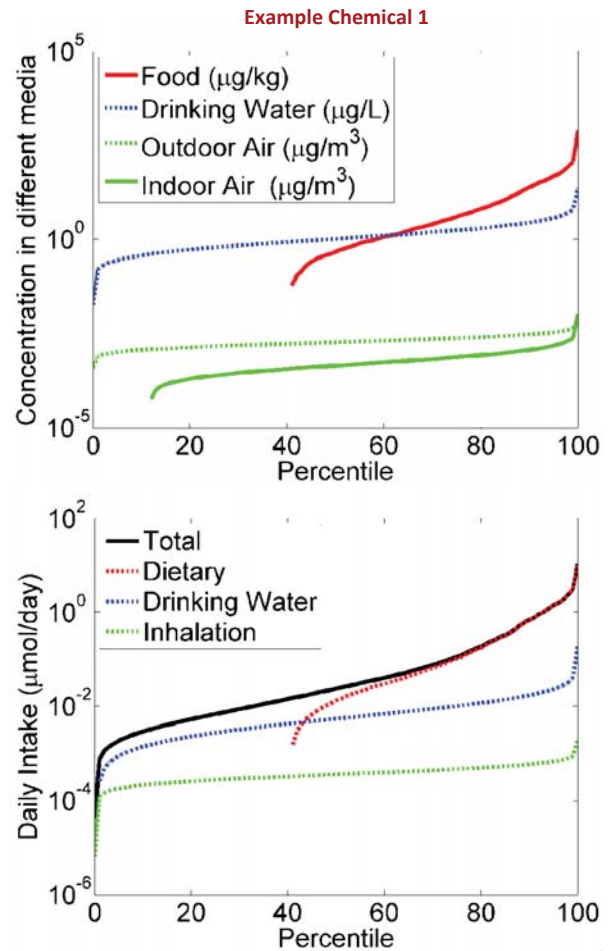
[†] Modeling Environment for Total Risk studies; development supported by USEPA, ATSDR, USDOE, NJDEP, ACC, and other government and private agencies.

Examples of "Tier 1" exposure rankings



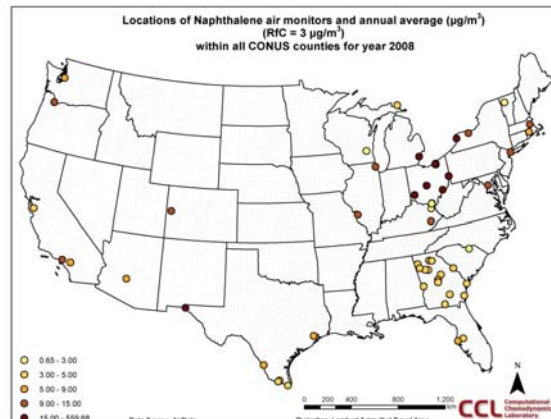
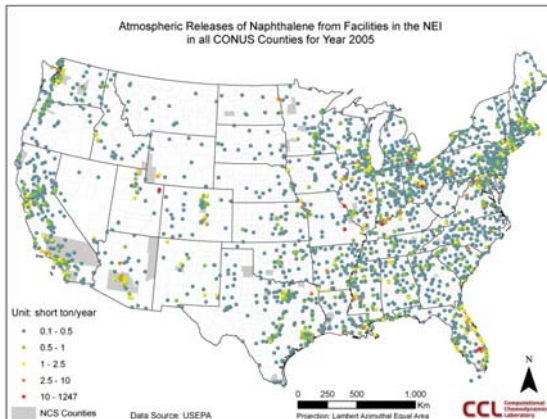
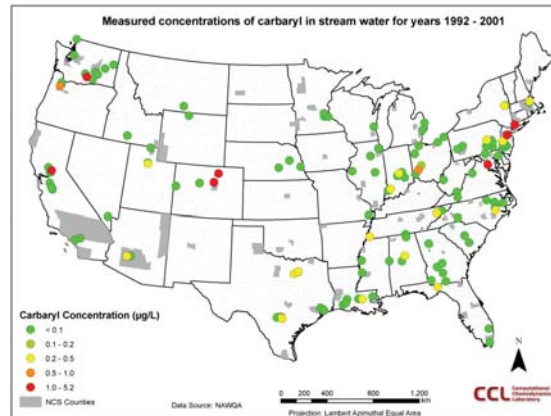
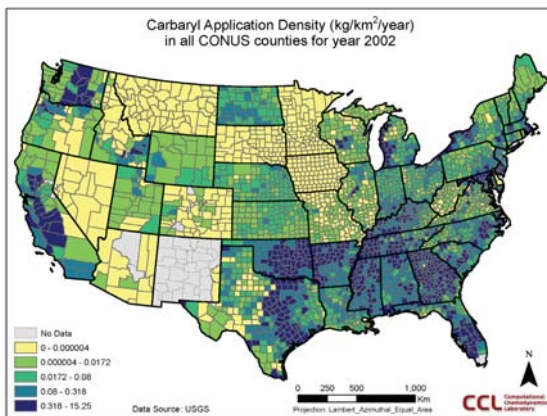
“Tier 2” exposure ranking

- “Tier 2” estimates are based on:
 - Different exposure factors sampled from national distributions for the general US population
 - inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.
 - Concentrations of the chemical in multiple media sampled from national measured distributions
 - ambient monitoring data
 - nationally representative field studies
 - contributions from environmental tobacco smoke are not considered in “Tier 2” exposure characterization
- Metrics considered
 - Percentage of population above a threshold average daily intake
 - 0.1 $\mu\text{g}/\text{day}$ and 1.0 $\mu\text{g}/\text{day}$
 - Different percentiles of intakes for the general US population
 - 10th percentile, median, and 90th percentile



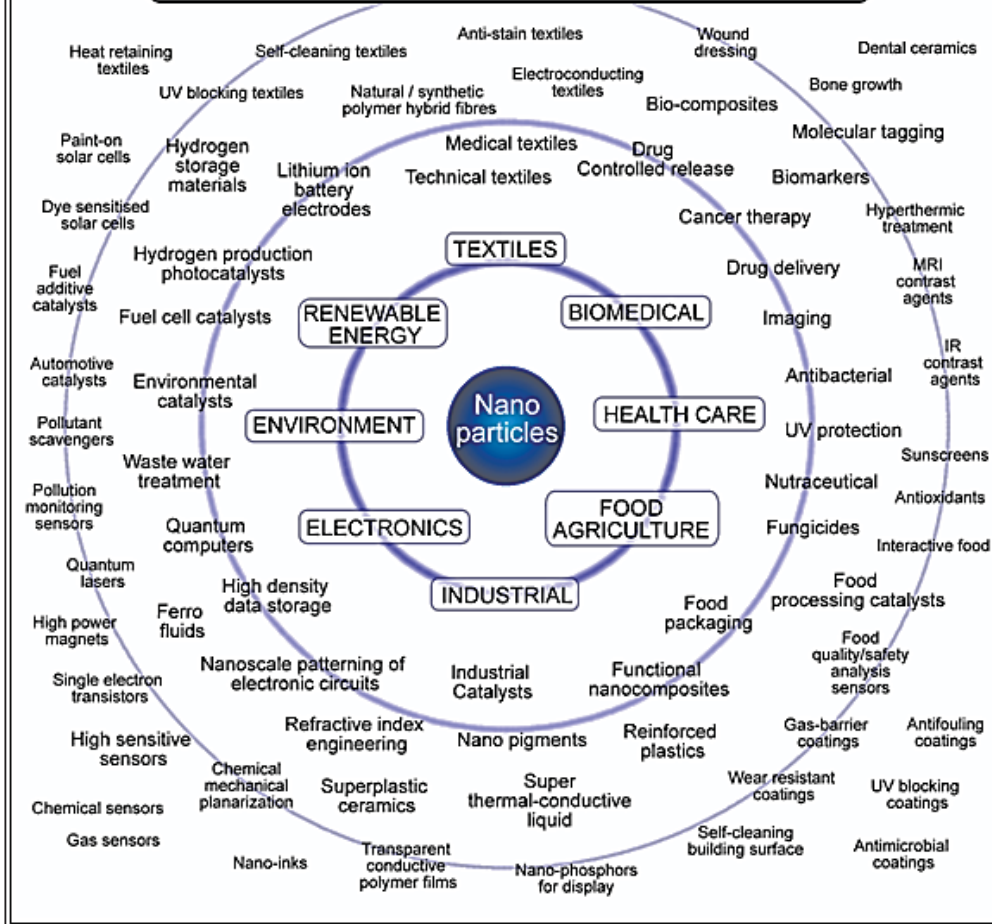
15

Examples of inputs used in PRoTEGE for exposure ranking: Releases and ambient levels of selected chemicals



16

APPLICATIONS OF NANOPARTICLES

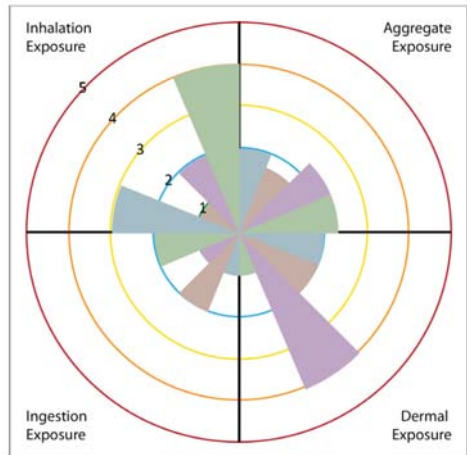


Nanoparticles are among the most challenging "Contaminants of Emerging Concern"

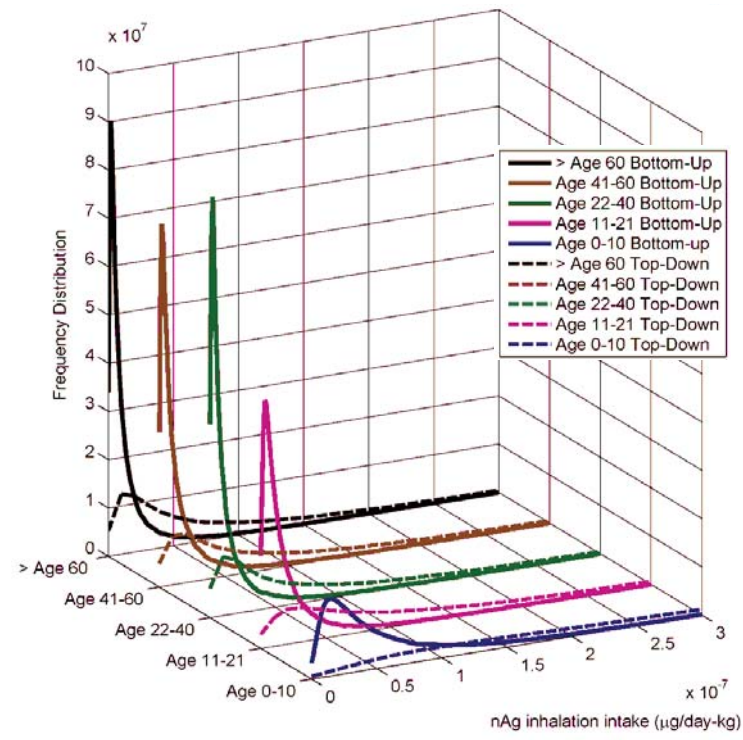
Assessments of human exposures and risks require a "Life-Cycle Analysis" approach: PROTEGE offers such a framework

Source: Tsuzuki (2009) *Int J Nanotechnology*

Preliminary PROTEGE-derived US-wide characterization of population inhalation exposure to silver nanoparticles (nAg) by age group

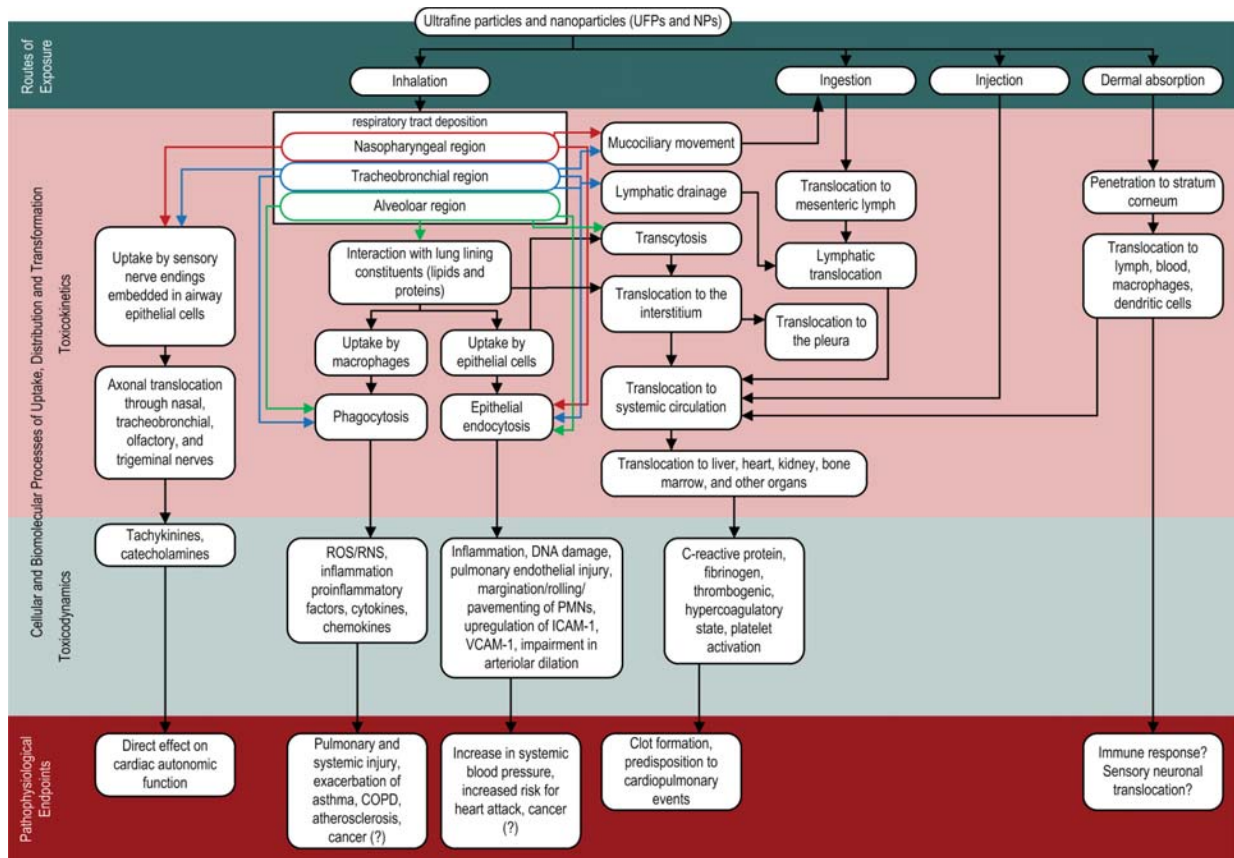


Semi-Quantitative Exposure Ranking				
	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	3	1	2	4
Ingestion	1	2	1	2
Dermal	2	2	4	1
Aggregate	2	1.66	2.33	2.33



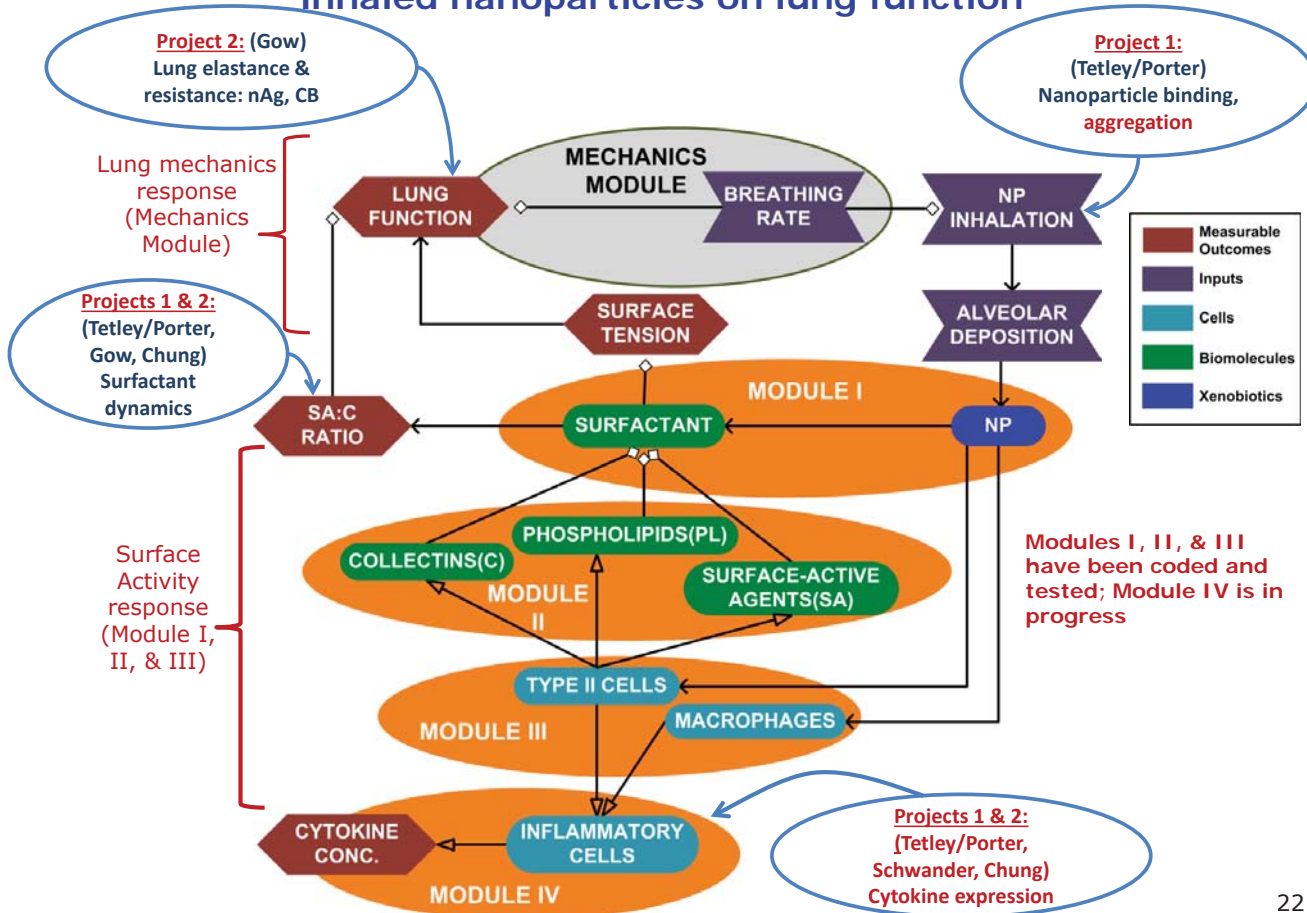
Predicted US population intake, by age group, of nAg from ambient air, employing bottom-up and top-down approaches

A modeling framework for assessing risk from "natural" and engineered ultrafine particles/nanoparticles in the environment



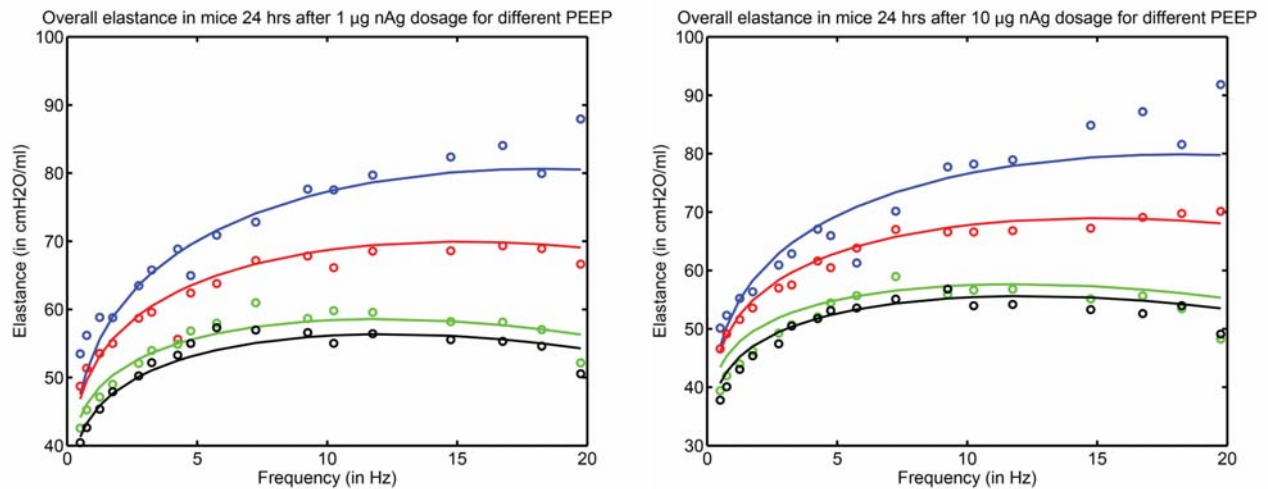
21

A modular mechanistic model quantifying effects of inhaled nanoparticles on lung function



22

Example model results compared to measurements of lung elastance



Measurements from Dr. Andrew Gow's lab.
Each data point is the mean of measurements from 12 mice

PEEP = Positive End Expiratory Pressure

23

Concluding Comments

- **ORC is committed to supporting regulatory needs of the State of NJ and related NJDEP activities**
- **A range of novel modeling and analysis tools have been developed at ORC/CCL to complement and extend "standard" platforms, and are being applied to a wide range of environmental problems**
 - Applications involve not only ozone, but also inhalation (and total) exposures to PM, air toxics, bioaerosols, "natural" and engineered nanoparticles, and multimedia contaminants (pesticides, solvents, heavy metals, etc.) in the ambient and in confined environments and microenvironments
 - Multiple "standard" modeling tools are used in applications (MM5, RAMS, HYPACT, HYSPLIT, M3/CMAQ, CAMx, ASPEN, AERMOD, HPAC, FLUENT, CFX; etc.)
 - Databases have been assembled and structured to facilitate comprehensive multivariate spatiotemporal analyses of environmental and demographic factors
 - A comprehensive and extensible new modeling framework (MENTOR) has been designed and implemented collaboratively with USEPA
 - A screening platform using simplified components of MENTOR and employing a Life Cycle Approach, PRoTEGE (Prioritization/Ranking of Toxic Exposures with GIS Extension), is under ongoing development with special focus on characterizing exposures/risks associated with Contaminants of Emerging Concern (CEC)
- **The "One Atmosphere" is evolving into the "One Environment" model; "Person Oriented Modeling" and "Life Cycle Analysis" are central in this approach**
 - These concepts are 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

24

Acknowledgements

Current and Recent Research Projects Relevant to the ORC Mission

- NJ DEP
 - Base funding for the Ozone Research Center (ORC) at EOHSI
- NIH/NIEHS/NIOSH
 - Center for Environmental Exposure and Disease (CEED) at EOHSI
 - National Children's Study (NCS)
 - Respiratory Effects of Silver and Carbon Nanomaterials (RESAC)
 - Cancer Among WTC Responders: Enhanced Surveillance, Exposure Assessment, and Cancer Specific Risk
- 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

25

Acknowledgements

- The CCL Team
 - Panos G. Georgopoulos
 - Jocelyn Alexander
 - Kristin Borbely
 - Teresa Boutillette
 - Linda Everett
 - Zhong-Yuan "Wheat" Mi
 - Christos Efstathiou *
 - Dwaipayan Mukherjee
 - Steven Royce
 - Alan Sasso *
 - Pamela Shade
 - Spyros Stamatelos *
 - Shu Xu
 - Xiaogang Tang
 - Yong Zhang
- NJDEP Collaborators
 - 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
 - Michael Ku
 - Winston Hao
 - Kevin Civerolo

*PhD awarded 2009-11

26

Supplemental Slides

27

A brief history of the Ozone Research Center at EOHSI

- **Established in 1989 with base funding from NJDEP**
 - Paul J. Lioy first director; Panos G. Georgopoulos was recruited and joined in Fall 1989 as deputy director and technical coordinator; focus is on local/regional ozone issues
 - Urban/mesoscale modeling capability (with UAM-IV, RPM-V etc.) established in 1990 on Princeton/GFDL computers (only two groups in the NE US with such capabilities then)
 - First graduate students (E. Short, A. Roy) recruited in 1991
 - First ORC science workshop held in 1993; held biannually since then (last in February 2011)
 - First external grants (USEPA STAR grants were awarded in 1992 and 1993)
 - First 5-year phase delivered long-term infrastructure; modeling support for the ozone SIP
- **During the 1994-2012 period ORC expanded significantly its focus and became the “core” for multiple national efforts focusing on developing and implementing source-to-dose-to-effect exposure analyses**
 - **Research evolved to include PM, air toxics, multimedia contaminants, biological mechanisms of exposure and effect, climatic change, nanoparticles, etc.**
 - **National recognition in various areas (uncertainty analysis; “person-oriented” (anthropocentric) exposure biology and assessment; integrative enviroinformatic and bioinformatic systems)**
 - Establishment of state-of-the art hardware/software capabilities (cluster computing)
 - Establishment of Center of Exposure and Risk Modeling (CERM) and of Environmental and Bioinformatics Computational Toxicology Center (ebCTC) with base funding from USEPA
 - Numerous relevant studies related to air pollution and inhalation exposure and dosimetry were pursued and completed (e.g. ACC-VOCs, NIEHS-WTC, NJDHSS-ACHILLES, NJ-OHSP-EI, etc.)
 - Dr. Shan He the regular collaborator and project officer from NJDEP
 - New and ongoing relevant studies include the National Children’s Study, CCAAD, RESAC, RAMNUC, NIOSH-WTC, etc.

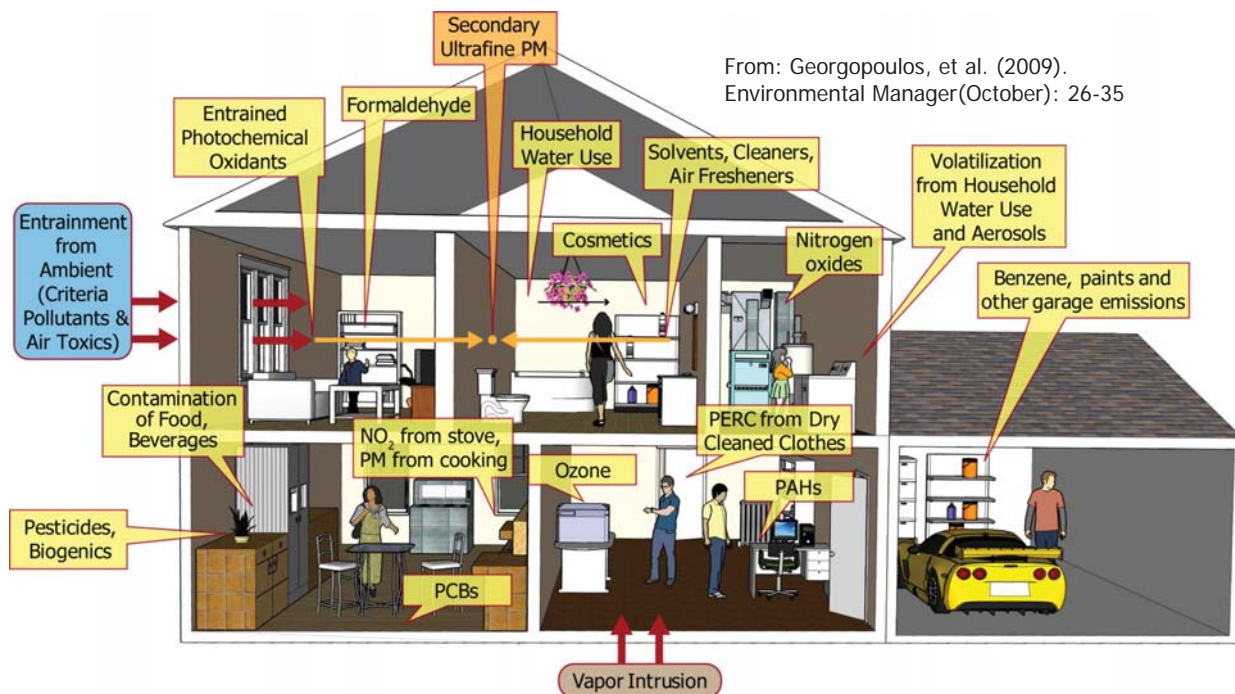
28

National Ambient Air Quality Standards (NAAQS)

Pollutant	Primary Standards			Secondary Standards		Attainment Status
	Level	Date	Averaging Time	Level	Averaging time	
CO	9 ppm	1971	8-hour	None		Attained
	35 ppm	1971	1-hour			
Lead	1.5 $\mu\text{g}/\text{m}^3$	1978	Quarterly Average	Same as Primary		Attained
	0.15 $\mu\text{g}/\text{m}^3$	2008	Rolling 3-Month Average	Same as Primary		Attained
NO ₂	53 ppb	1971	Annual	Same as Primary		Attained
	100 ppb	2010	1-hour	None		?
PM ₁₀	150 $\mu\text{g}/\text{m}^3$	1987	24-hour	Same as Primary		Attained
PM _{2.5}	15.0 $\mu\text{g}/\text{m}^3$	1997	Annual	Same as Primary		Attained
	35 $\mu\text{g}/\text{m}^3$	2006	24-hour	Same as Primary		Attained
	12.0 $\mu\text{g}/\text{m}^3$? 30 $\mu\text{g}/\text{m}^3$?	?	Annual 24-hour			Not Attaining
Ozone	120 ppb	1979	1-hour	Same as Primary		Attained
	80 ppb	1997	8-hour	Same as Primary		Attained
	75 ppb	2008	8-hour	Same as Primary		Not Attaining
	60 – 70 ppb ?	?				Not Attaining
SO ₂	30 ppb	1971	Annual	50 ppb	3-hour	Attained
	140 ppb	1971	24-hour			
	75 ppb	2010	1-hour	None		?

29

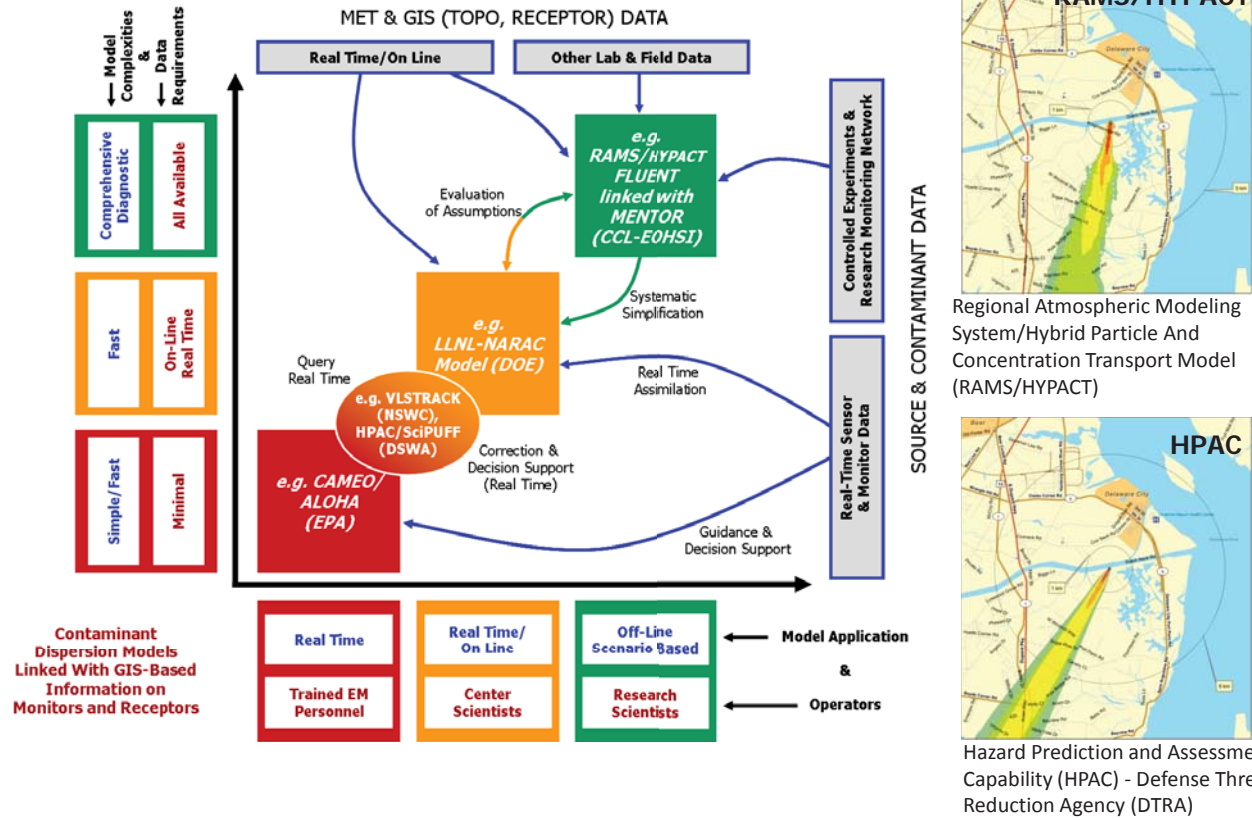
Often the most significant exposures to airborne contaminants take place in confined (residential and public) microenvironments



For most people the majority of exposures to airborne contaminants 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).

30

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



31

A health endpoint-specific inhalation Exposure Index

$$E_{\text{inhalation},i,p} = \left[\omega_{\text{toxics},p} \sum_{j=1}^{N_{\text{toxics},p}} \frac{\overline{C_{i,j}}}{\text{RfC}_{j,p}} + \omega_{\text{crit},p} \sum_{k=1}^{N_{\text{crit},p}} \left(\frac{\int_{\tau_1}^{\tau_2} C_{i,k}(t) dt}{(\tau_2 - \tau_1)} \times \frac{1}{\text{RpC}_{k,p}(\tau_2, \tau_1)} \right) \right] \times \omega_{\text{pop},i,p}$$

where:

- $E_{\text{inhalation},i,p}$ inhalation exposure index of segment i in relation to endpoint p
- i geographic region of concern (e.g. segment or county)
- p endpoint of concern (e.g. respiratory effects)
- $\overline{C_{i,j}}$ average concentration of the air toxic j in area i
- $C_{i,k}(t)$ average concentration of criteria pollutant k in area i
- τ_1 and τ_2 start and end of averaging period for concentrations of criteria pollutant k in area i
- $\omega_{\text{toxics},p}$ relative weight of air toxics in relation to endpoint p
- $\omega_{\text{crit},p}$ relative weight of criteria pollutants considered in relation to endpoint p
- $\omega_{\text{pop},i,p}$ target population weight of segment i in relation to endpoint p (e.g. fraction women of child bearing age)
- $N_{\text{toxics},p}$ number of air toxics considered in relation to endpoint p
- $N_{\text{crit},p}$ number of criteria pollutants considered in relation to endpoint p
- $\text{RfC}_{j,p}$ reference concentration for air toxic j in relation to endpoint p
- $\text{RpC}_{k,p}(\tau_1, \tau_2)$ a reference concentration for criteria pollutant k in relation to endpoint p for averaging period between τ_1 and τ_2

32








Air pollutants used for the inflammation-specific inhalation Exposure Index

An endpoint specific Inhalation Exposure Index was calculated for the "inflammatory" criteria pollutants (ozone, PM_{2.5}, NO₂, SO₂) and the following HAPs (air toxics):

- acetaldehyde
- acrolein
- acrylic acid
- acrylonitrile
- antimony compounds
- beryllium compounds
- Bis(2-ethylhexyl) phthalate
- Chlorine
- 2-Chloroacetophenone
- Chloroprene
- Chromium VI compounds
- Cobalt compounds
- 1,3-Dichloropropene
- Diesel emissions
- Diethanolamine
- Epichlorohydrin
- 1,2-Epoxybutane
- Ethylene dibromide
- Ethylene glycol
- Formaldehyde
- Hexachlorocyclopentadiene
- Hexamethylene-1,6-diisocyanate
- Hydrochloric acid
- Maleic anhydride
- Methyl bromide
- Methyl isocyanate
- Methyl methacrylate
- Methylene diphenyl diisocyanate
- Naphthalene
- Nickel compounds
- Nitrobenzene
- Phosgene
- Phthalic anhydride
- Propionaldehyde
- Propylene dichloride
- Propylene oxide
- Styrene oxide
- Titanium tetrachloride
- Toluene
- 2,4-Toluene diisocyanate
- Triethylamine
- Vinyl acetate

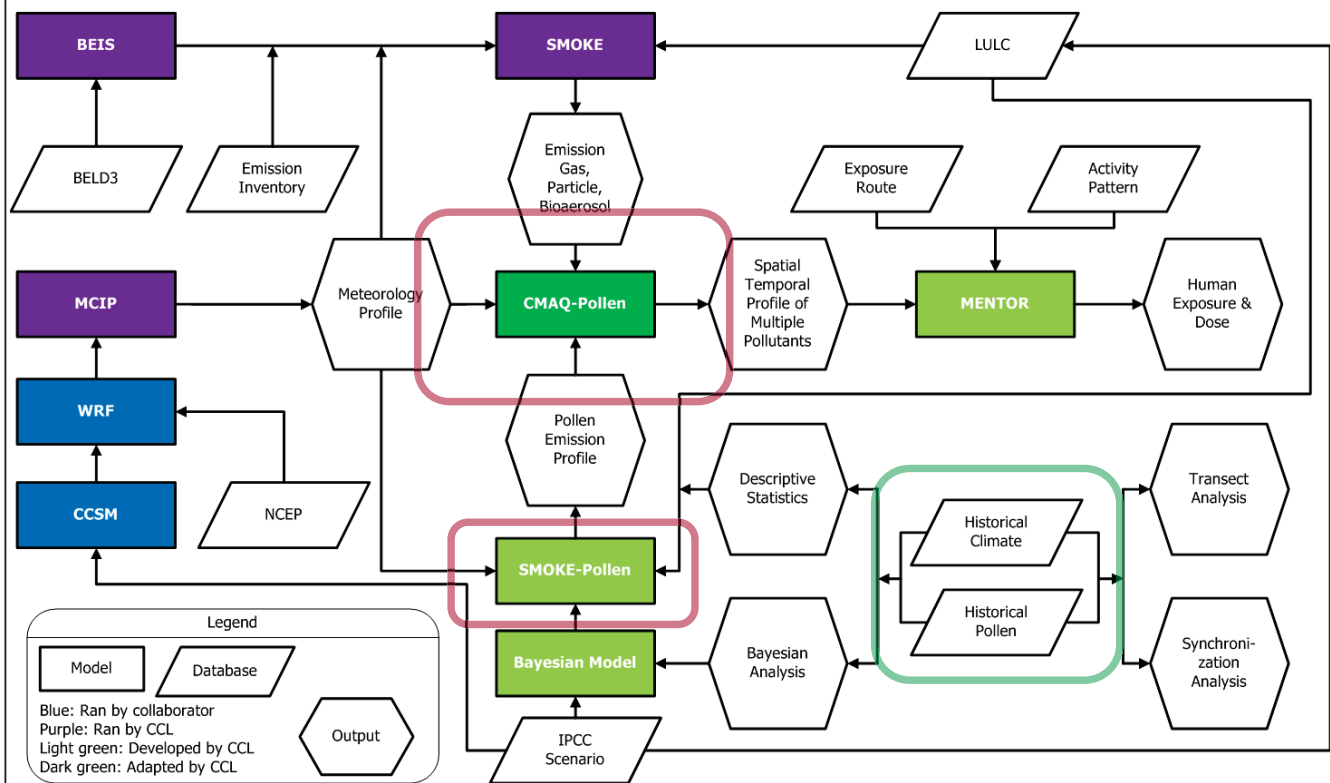
33

Allergenic tree pollen species, particle diameters, pollen shedding periods, and spatial coverage densities as reported in the Biogenic Emission Landuse Database (BELD³).

	FAMILY	MAJOR SPECIES	Dp (µm)	POLLEN PERIOD	ALLERGEN	OTC BELD3 density (%)
	<i>Quercus</i>	Oaks	19-39	March - June	t7	32.35
	<i>Pinaceae</i>	Pines	53-73	May - June	t16, t73	9.44
	<i>Cupressaceae</i>	Cypress, Juniper, Cedar	20-36	April - May	t6, t17, t23	3.64
	<i>Moraceae</i>	Mulberries	11-25	March - June	t70	< 1
	<i>Betulaceae</i>	Alder, Birch, Hazel	19-32	April - May	t2, t3, t4, t210	3.42
	<i>Oleaceae</i>	Ashes	26-33	March - May	t9, t15	3.15
	<i>Fagaceae</i>	Beech	40-44	May-June	t5	4.80
	<i>Aceraceae</i>	Maples	23-38	April - May	t1	13.90
	<i>Carya</i>	Hickory, Pecan	35-55	May - June	t22	3.64

34

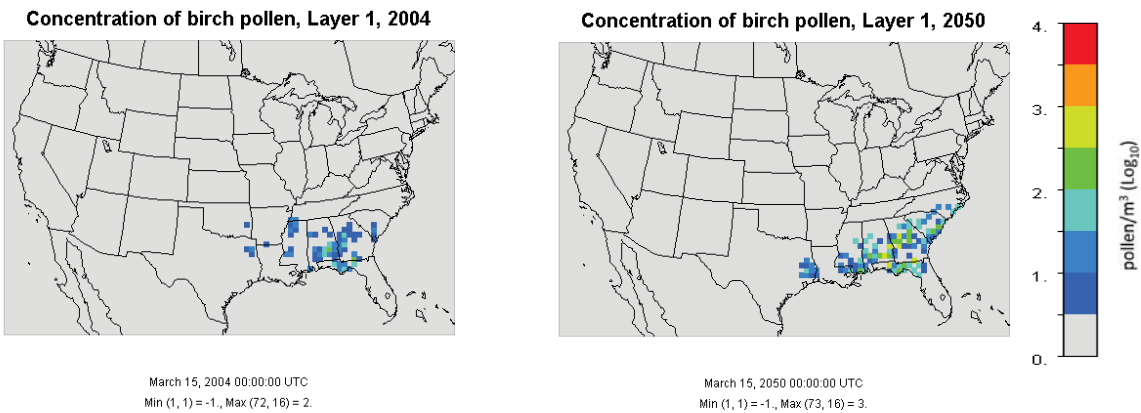
Overview of the WRF-SMOKE-CMAQ-Pollen modeling system



A modeling system linking climate change and exposure

Spatiotemporal concentration profiles of birch pollen, Layer 1

- Domain: Contiguous US
- Period: March 15th 00:00 – April 25th 23:00
- Resolution: 50 x 50 km; Hourly; 10 Layers



Layers are based on pressure

- Layer 1: 0-59m above the ground surface
- Layer 10: 1800m and more above the ground surface