AGENDA
Technical Symposium
Scientific Basis of Air Quality Modeling for the San Joaquin Valley 2012 PM2.5 Plan

April 27, 2012
10:00 a.m. – 12:30 p.m.

1. **Introductions and Opening Remarks**
Mr. Samir Sheikh, Director
Strategies and Incentives
San Joaquin Valley Air Pollution Control District

Ms. Lynn Terry, Deputy Executive Officer
California Air Resources Board

2. **Overview of PM2.5 Plan Development**
Ms. Jessica Fierro, Supervisor
Plan Development
San Joaquin Valley Air Pollution Control District

3. **Nature of PM2.5 in the San Joaquin Valley**
Ms. Karen Magliano, Chief
Air Quality Data Branch
California Air Resources Board

4. **Review of Modeling Results from CRPAQS**
Dr. Michael Kleeman, Professor
Department of Civil and Environmental Engineering
University of California, Davis

5. **Modeling for SIP Purposes**
Mr. John DaMassa, Chief
Modeling and Meteorology Branch
California Air Resources Board

6. **Technical Approach for 2012 SJV PM2.5 Plan Modeling**
Dr. Ajith Kaduwela, Manager
Regional Air Quality Modeling Section
California Air Resources Board

7. **Question and Answer Session**

Technical Symposium

Scientific Basis of Modeling for the SJV 2012 PM2.5 Plan

San Joaquin Valley Air District
California Air Resources Board

April 27, 2012

Agenda

- Introductions and Opening Remarks
- Overview of PM2.5 Plan Development
- Nature of PM2.5 in the San Joaquin Valley
- Review of Modeling Results from CRPAQS
- Modeling for SIP Purposes
- Technical Approach for 2012 SJV PM2.5 Plan Modeling
- Question and Answer Session
  - During this workshop, webcast participants can email questions to: webcast@valleyair.org

Overview of PM2.5 Plan Development

Jessica Fierro, Plan Development Supervisor
San Joaquin Valley Air District

Introduction to the *2012 PM2.5 Plan*

- Plan for addressing EPA's 24-hour PM2.5 standard of 35 µg/m³, as set in 2006
- Plan goals:
  - Meet federal requirements
  - Assure expeditious attainment of the standard
  - Evaluate the benefits of the significant emissions reductions that will be achieved between now and 2019 under current regulations
  - Put together the strongest plan possible, with the strongest feasible control measures

SJV PM2.5 Plan Schedule

Plan for addressing EPA's 24-hour PM2.5 standard of 35 µg/m³, as set in 2006:

- Ongoing: Scientific research, technical analyses, outreach
- April: First round of public workshops
  - April 27: District/ARB Technical Symposium on the Scientific Basis of PM2.5 Plan Modeling
  - April 30: District workshop on general plan direction
- June & August: revised drafts, workshops
- October 2012: District plan adoption
- November 2012: ARB plan adoption
- December 14, 2012: Plan due to EPA

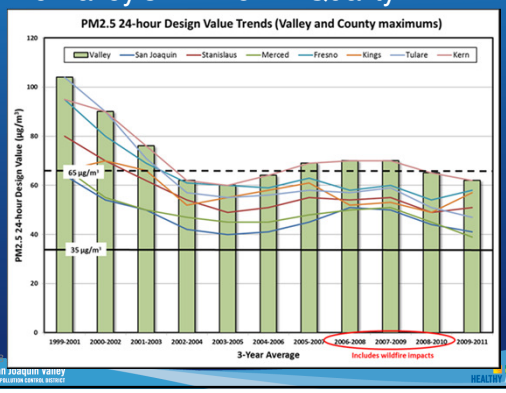
Plan Requirements

- **Analysis of PM2.5 concentrations**
- **Emissions inventories**
- **Photochemical modeling and Weight of Evidence analyze future air quality and identify emission reduction for attainment**
- Emission control strategies
- Transportation conformity budgets
- Reasonable Further Progress demonstration
- Contingency measures

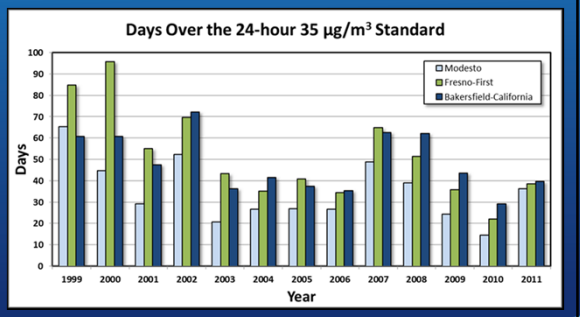
The Valley's PM2.5 Air Quality

- Evaluating multiple parameters provides broader picture of air quality progress
  - "Design values:" the attainment test; 3-year averages following EPA protocols
  - "Exceedances days" (24-hr average greater than 35 µg/m^3)
  - Air Quality Index (AQI) Trends
  - Concentrations by hour, day, and season
- Speciated data to determine types of PM contributing to total concentrations

The Valley's PM2.5 Air Quality



The Valley's PM2.5 Air Quality



Emissions Inventory

- Best available estimates of the amount of pollutants and precursors being emitted from each source type
- Inventories continuously improved
- Plan's inventory is a snapshot reflecting best information at the time for use in modeling & control measures evaluation
- District coordinating closely with ARB to ensure accuracy

Improvements to Base Year Emission Inventory

- Point source emissions are based on District reports for 2007
- Mobile source emission estimates reflect all adopted ARB rules and the latest activity assumptions
- Key stationary and area source categories reflect economic recession, newer activity data, and/or updated emission factors

Emission Inventory Forecasts

- Forecasts to future years are essential in demonstrating attainment and maintenance of the air quality standards
- The key components are:
  - Base Year Inventory – the best estimate of current emissions
  - Growth Factors – an estimate of the annual growth or decline in the activity for each source category
  - Control Factors – an estimate of the emission reductions from adopted rules and regulations targeting specific source categories

Nature of PM2.5 in the San Joaquin Valley

Karen Magliano
California Air Resources Board
Technical Symposium
April 27, 2012

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PM Characterization

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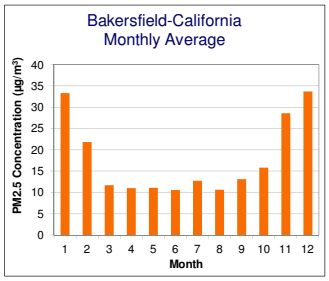
High PM2.5 Levels Occur In Winter

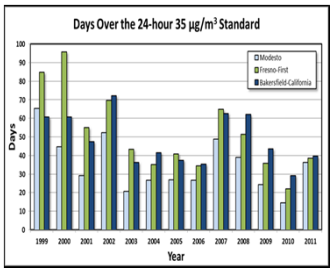


- PM2.5 builds up over several days or weeks (episode)
- Episodes generally occur during periods with:
  - stagnation
  - cool temperatures
  - high humidity
  - low mixing depths

3

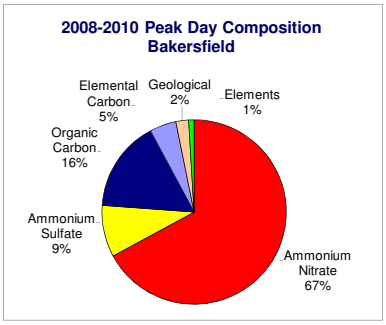
4

Challenge of 24-Hour Standard



- Focuses on most severe days
- Strongly influenced by meteorology
- Impacts of episodic emissions such as residential wood burning

Monitored PM2.5 Chemical Components



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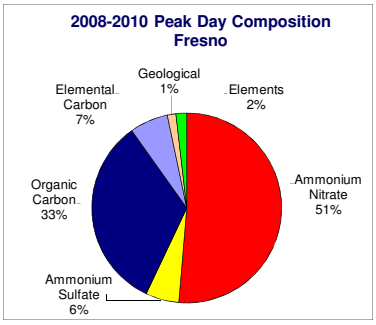
Monitored PM2.5 Chemical Components



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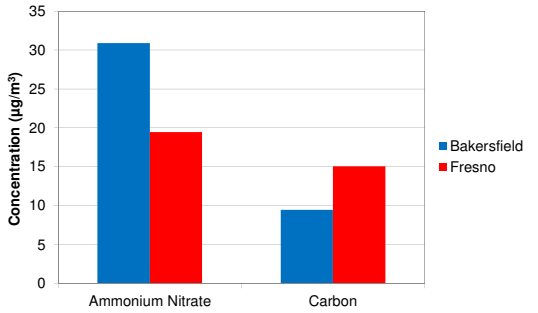
Monitored Concentrations of Key Species



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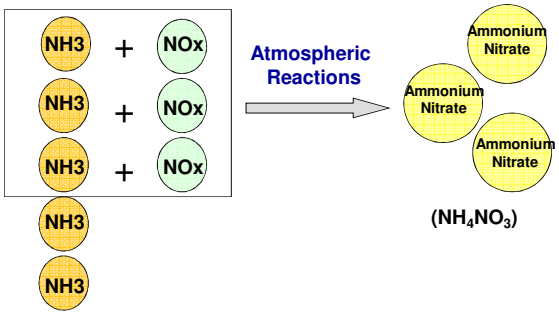
Ammonium Nitrate Formation (Excess Ammonia)



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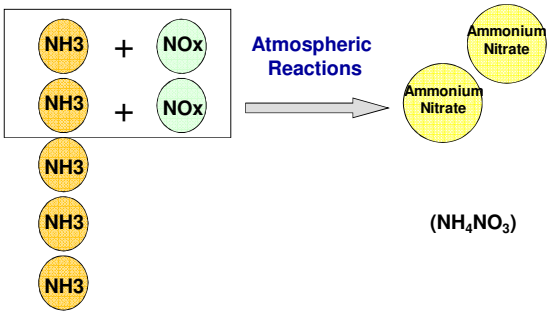
Ammonium Nitrate Formation (NOx Control)



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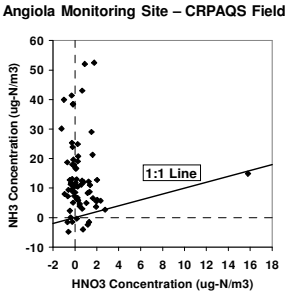
Measured Ammonia Much More Abundant than Nitric Acid



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Linkage to Modeling

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Role of Air Quality Data in Attainment Demonstration

- Calculate design values
- Select modeling base year
- Weight of Evidence

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Design Value Calculation

- Defines air quality starting point
- Uses measured PM2.5 concentrations
- Based on 98th percentile (generally between the 2nd and 8th highest value)
- Calculated as 3-year average

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Selecting Base Year For Planning

- Appropriate base year considers air quality and meteorology
- Base year with stagnant meteorology is a conservative approach
- Attainment demonstration estimates change in design value between base year and attainment year

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2007 Base Year

- 2007 meteorology one of most conducive to PM2.5 formation
- Includes various types of meteorology conducive to high PM2.5
- 2007 PM2.5 98th percentile concentrations highest in recent years
- Excludes influence of 2008 wild fires

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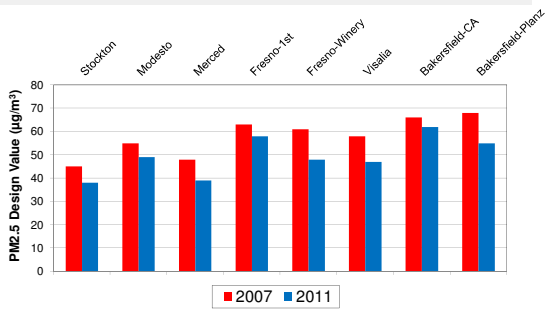
Design Values*



* Year assigned to design value reflects last year of three year period

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Weight of Evidence

- Attainment demonstration based on weight of evidence approach
- Collective assessment of control approach based on:
  - air quality grid modeling
  - source-receptor modeling
  - observed air quality trends
  - emission trends
  - field/modeling studies

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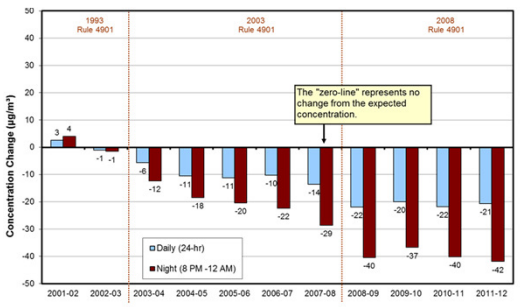
Effectiveness of Wood Burning Controls



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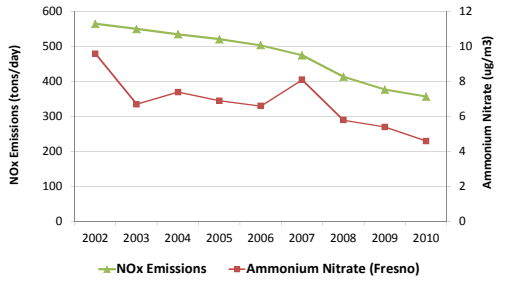
Effectiveness of NOx Controls



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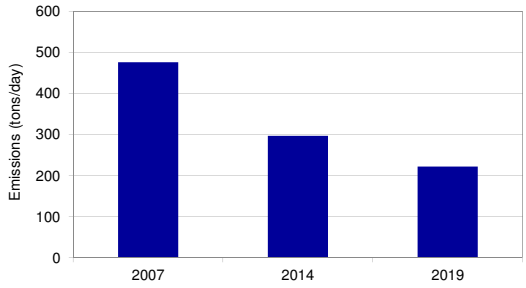
Future NOx Emission Trends



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Fine Particulate Matter in the San Joaquin Valley: Review of Modeling Results From CRPAQS

Michael Kleeman
Civil and Environmental Engineering, UC Davis

Mechanistic Air Quality Models

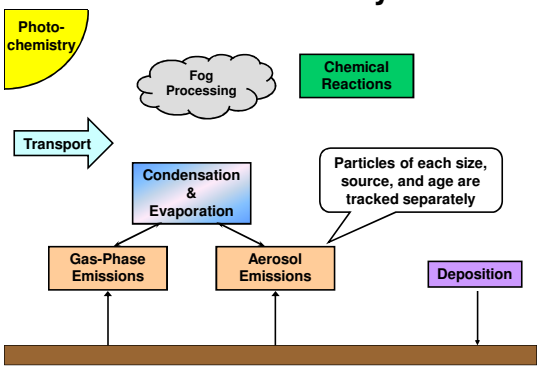


Figure courtesy of Prakash Bhave, U.S. EPA

Chemical Mechanism

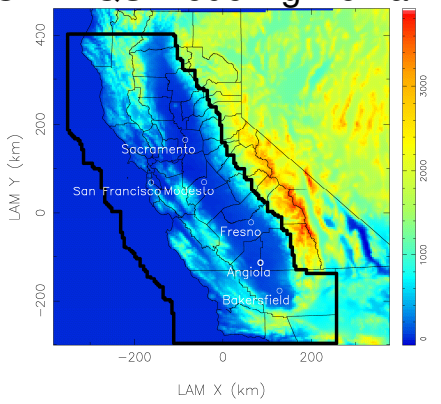
335 Active Species

15 Steady State Radicals

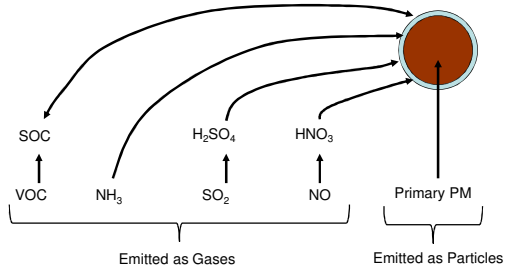
1500 Chemical Reactions

+300,000 grid cells

CRPAQS Modeling Domain



Basic Particle Chemistry



VOC = Volatile Organic Compounds (benzene, ethanol, formaldehyde, …)
SOC = semi-volatile organic compounds (mostly unknown)
Primary PM = particulate matter emitted directly from sources (trace metals – aluminum, silicon, iron, nickel, etc, elemental carbon, organic carbon)

CRPAQS PM2.5 Mass

Black Line – measurements

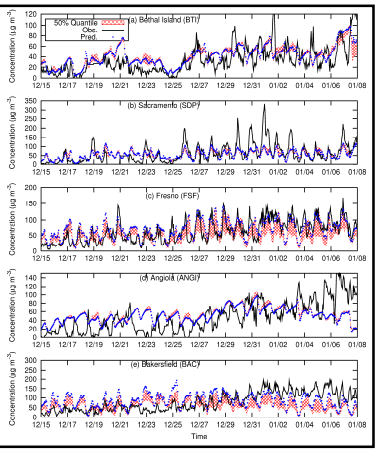
Blue Line – predictions

Red Shading – Mid 50% Quantile within 10km of monitor

Major trends are captured at most stations

Under-prediction of mass at Angiola and Bakersfield near the end of the episode

Source: Q. Ying, J. Lu, P. Allen, P. Livingstone, A. Kaduwela, and M. Kleeman "Modeling Air Quality During the California Regional PM10/PM2.5 Air Quality Study (CRPAQS) Using the UCD/CIT Source-Oriented Air Quality Model – Part I. Base Case Model Results.", Atmos. Env., 42, pg8954-8966, 2008.

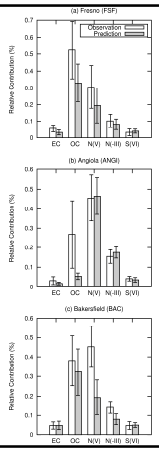


Relative Component Contributions to PM

Average and standard deviation of predictions and observations is based on 55 samples

Urban locations (Fresno and Bakersfield)
Predictions and observations match except for nitrate under-prediction at Bakersfield

Rural location (Angiola)
OC under-prediction. What primary sources are we missing? What SOA formation mechanisms are we missing?



Source: Q. Ying, J. Lu, P. Allen, P. Livingstone, A. Kaduwela, and M. Kleeman "Modeling Air Quality During the California Regional PM10/PM2.5 Air Quality Study (CRPAQS) Using the UCD/CIT Source-Oriented Air Quality Model – Part I. Base Case Model Results.", Atmos. Env., 42, pp8954-8966, 2008.

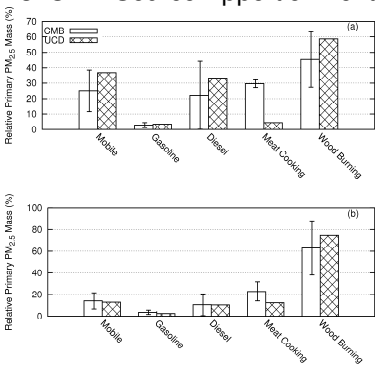
Grid Model vs. CMB Source Apportionment

Angiola

**Dust sources removed from grid model

Fresno

**Dust sources removed from grid model



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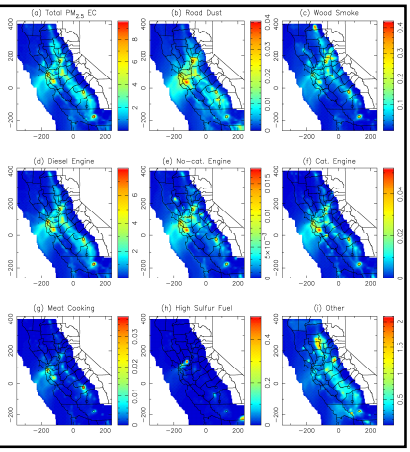
Regional EC Source Contributions

Urban hotspots

Diesel dominates



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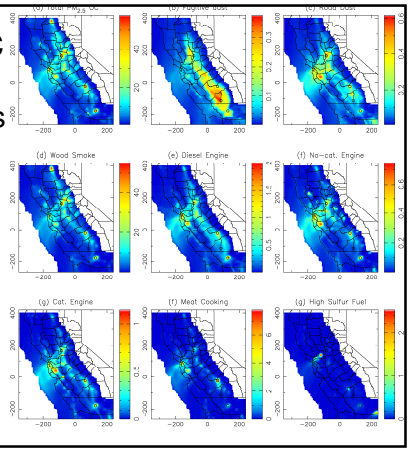
Regional OC Source Contributions



Urban hotspots

Wood smoke dominates

Source: Q. Ying, J. Lu, A. Kaduwela, and M. Kleeman "Modeling Air Quality During the California Regional PM10/PM2.5 Air Quality Study (CRPAQS) Using the UCD/CIT Source-Oriented Air Quality Model – Part II. Regional Source Apportionment of Primary Airborne Particulate Matter.", Atmos. Env., 42, pp8967-8978, 2008.

Spectrum of Reactive Nitrogen Compounds

- NO, NO2, NO3, N2O5, HONO, PAN, HNO3

Direct Emissions

Reactive Intermediate Products

Stable End Product From Atmospheric Chemistry

- $HNO_3 + NH_3 \rightarrow NH_4NO_3$

Direct Emissions

Particle Phase Nitrate

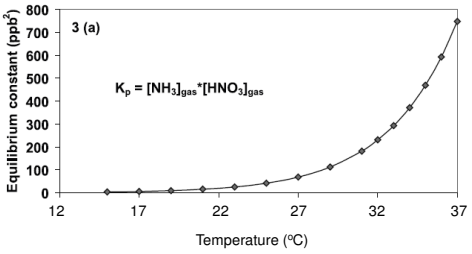
Nighttime/Winter Nitrate Formation

- $NO \xrightarrow{O_3} NO_2 \xrightarrow{O_3} NO_3 \rightarrow N_2O_5 \xrightarrow{H_2O} 2HNO_3$

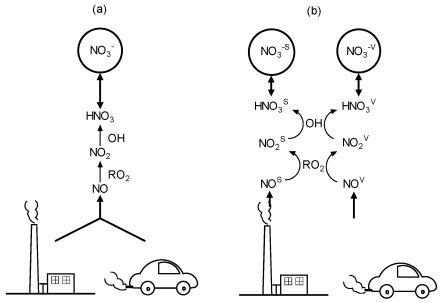
- Main oxidant is O_3 – favors low sunlight intensity, wet conditions

Equilibrium Dissociation Constant for Ammonium Nitrate

Ammonium nitrate will not form when $[NH_3]*[HNO_3] < Kp$

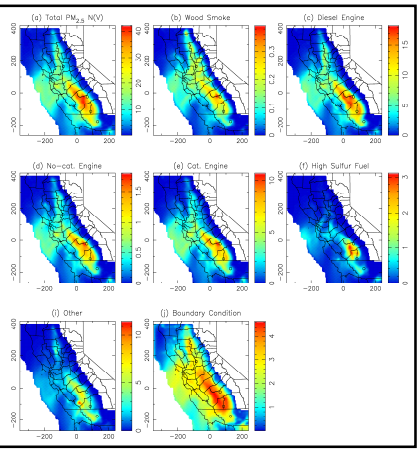


Source Apportionment of Secondary PM

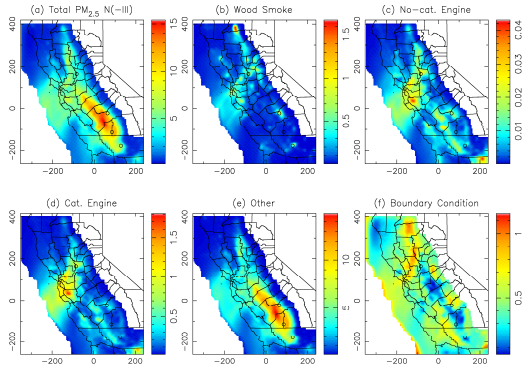


Source: Ying, Q. and M.J. Kleeman. "Source contributions to the regional distribution of secondary particulate matter in California." Atmospheric Environment, Vol 40, pp 736-752, 2006.

Regional Nitrate Source Contributions

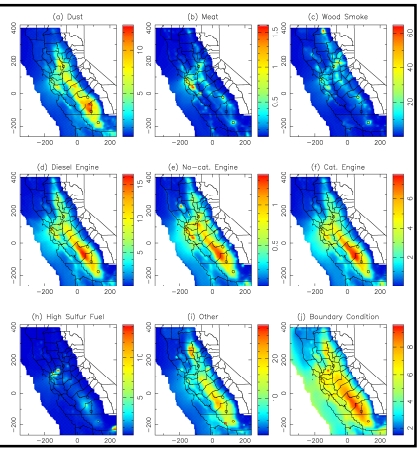


Regional NH4+ Source Contributions



Source: Q. Ying, J. Lu, A. Kaduwela, and M. Kleeman "Modeling Air Quality During the California Regional PM10/PM2.5 Air Quality Study (CRPAQS) Using the UCD/CIT Source-Oriented Air Quality Model – Part III. Regional Source Apportionment of Secondary and Total Airborne PM2.5 and PM0.1.", Atmos. Env., 42, pp8967-8978, 2008.

Regional PM2.5 (primary + secondary) Source Contributions



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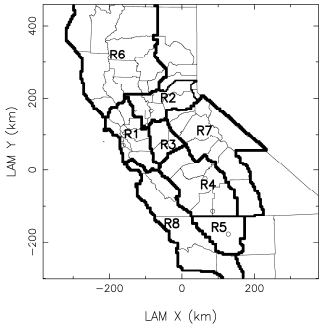
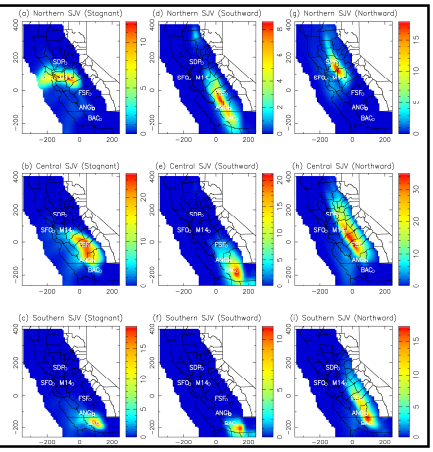
How Much PM Does Each Region Contribute to Other Regions?



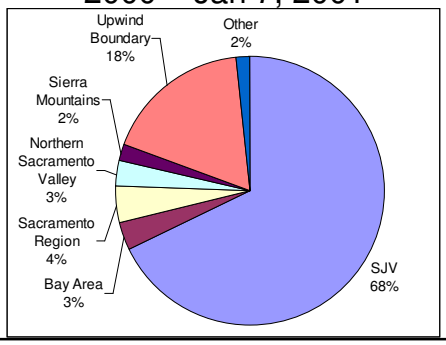
Source: Q. Ying, and M. Kleeman "Regional Contributions to Airborne Particulate Matter in Central California During a Severe Pollution Episode", Atmos. Env., 43, 1218-1228, 2009.

PM2.5 Nitrate

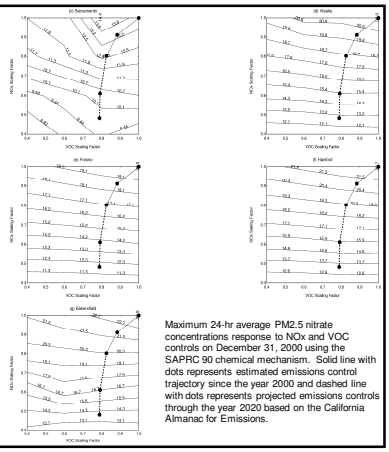


Source: Q. Ying, and M. Kleeman "Regional Contributions to Airborne Particulate Matter in Central California During a Severe Pollution Episode", Atmos. Env., 43, 1218-1228, 2009.

Regional Contributions to SJV PM2.5 Nitrate Between Dec 15, 2000 – Jan 7, 2001

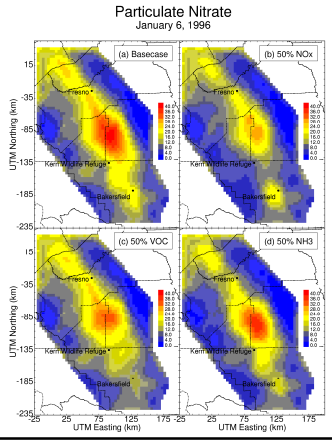


Nitrate Control Options



Maximum 24-hr average PM2.5 nitrate concentrations response to NOx and VOC controls on December 31, 2000 using the SAPRC 90 chemical mechanism. Solid line with dots represents estimated emissions control trajectory since the year 2000 and dashed line with dots represents projected emissions controls through the year 2020 based on the California Almanac for Emissions.

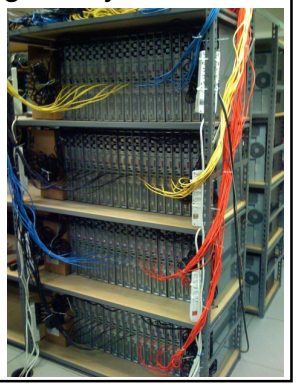
Control Strategy Effectiveness



Source: Kleeman MJ, Ying Q, Kaduwela A. Control strategies for the reduction of airborne particulate nitrate in California's San Joaquin Valley. Atmospheric Environment 39: 5325-5341, 2005.

Research vs. Regulatory Models

- Research Model
  - Develop new techniques
  - Emphasis on science questions
  - Usually increased computational burden
- Regulatory Model
  - Accepted techniques
  - Emphasis on practical application for SIP



Modeling for SIP Purposes

John DaMassa, Chief

Modeling and Meteorology Branch
Planning and Technical Support Division
California Air Resources Board

California Regional Particulate Matter Air Quality Study (CRPAQS)

- Major field study conducted in 2000
- Funded by a public / private partnership
- Provided the fundamental science behind the annual $PM_{2.5}$ plan and the current plan
- Provided the most comprehensive data and science in the country on understanding the origin and fate of $PM_{2.5}$
- Continues to be a cornerstone of $PM_{2.5}$ research

Consistency with U.S. EPA Guidance

- *"Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, $PM_{2.5}$, and Regional Haze"*
- Additional implementation guidance

Consistency with U.S. EPA Guidance

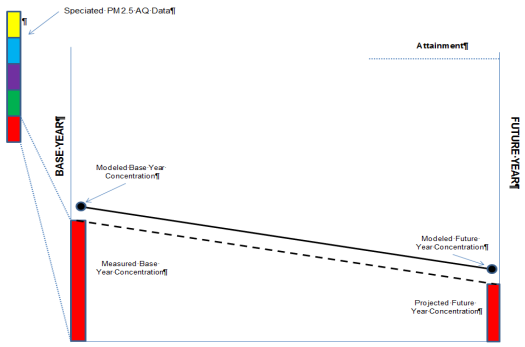
- Appropriate model(s) and other analyses
- Need for modeling protocol document
- Application and evaluation of model(s)
- Model attainment test
- Supplemental analyses
- Use of the best possible science

Weight of Evidence Approach for Attainment

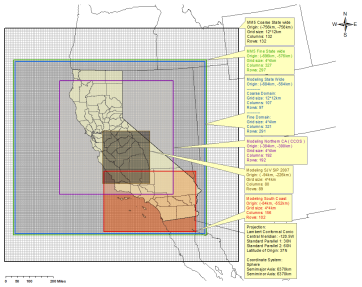
- Use all available technical information in a corroborative manner to determine best attainment strategy:
  - Grid-based photochemical modeling
  - Supplemental analyses:
    - Air quality trends
    - Emission trends
    - Source – receptor modeling (CMB, etc.)

Use and application of Photochemical Models

- Identifying the most effective mix of pollutants to control
- Establishing attainment targets
- Models are best used in a relative (rather than absolute) sense
  - Relative Response Factors (RRFs)
- Attainment test combines measures data and modeling to project air quality into the future
  - **S**peciated **M**odel **A**ttainment **T**est (SMAT)



Modeling Process



Modeling Process *(Meteorology)*

- Predict weather variables for every grid cell every few seconds for an entire year:
  - Temperature
  - Winds
  - Relative humidity
  - Stability
  - Pressure
  - Many more…
- Runs can take months

Modeling Process *(Air Quality)*

- Predict air quality for every grid cell every few seconds for a year
- Predict all components of $PM_{2.5}$:
  - *EC*
  - *OC*
  - *Ammonium nitrate*
  - *Ammonium sulfate*
  - *Others*
- Primary and secondary contributions
- Individual runs can take weeks

Modeling Process *(Quality Assurance)*

- Does the model replicate the observed nature of the $PM_{2.5}$ problem?
- Requires:
  - Iterative model runs
  - Re-generating meteorology and emissions inputs
  - Evaluating predictions for each specie
  - Focus evaluation on seasons / months contributing to high $PM_{2.5}$

Science Review

- Preparation of modeling protocol
- Peer review
- Stakeholder workshops
- Ongoing, thorough QA/QC throughout modeling process
- Board hearings

Ongoing Efforts to Improve Science

- Annual science meetings:
  - *International Conference on Atmospheric Chemical Mechanisms*
  - *International Aerosol Modeling Algorithms Conference*
- Field studies to improve modeling databases:
  - *U.S. EPA / ARB Advanced Monitoring Initiative (Feb. 2007)*
  - *ARCTAS (June 2008)*
  - *CalNex (May-July 2008)*
  - *DiscoverAQ (Jan-Feb 2013)*

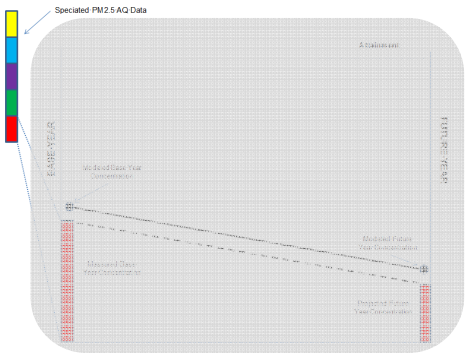
Technical Approach for 2012 SJV $PM_{2.5}$ Plan Modeling

Ajith Kaduwela, Ph.D.

Modeling and Meteorology Branch
Planning and Technical Support Division
California Air Resources Board

Outline of the Presentation

- Construction of the speciation for Federal Reference Method (FRM) filters
- Calculation of the future Design Value
- Meteorological and photochemical modeling
- Limiting precursors and their efficacies
- Resource requirements
- Current status of modeling

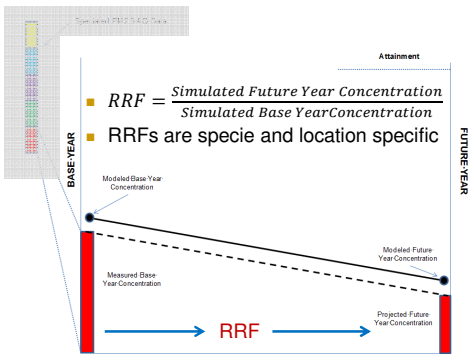


"Speciating" the FRM Filter

- Speciated Model Attainment Test (SMAT), which uses RRF, requires speciated $PM_{2.5}$
- Federal Reference Method (FRM) filters are not speciated
- Four FRM sites have co-located speciation monitors
- Use Sulfate, Adjusted Nitrate, Derived Water, Inferred Carbonaceous material balance approacH (SANDWICH) to estimate FRM speciation

Five things about SANDWICH

- Sulfate, EC, geologic – no adjustments
- Nitrate – use a thermodynamic equation to account for different nitrate collection efficiencies of speciation and FRM filters
- Water – use another thermodynamic equation to calculate particle-bound water
- Ammonium ion – calculated using ion balance of sulfates and nitrates
- Carbonaceous Material – use species mass balance to infer the mass of organic carbon

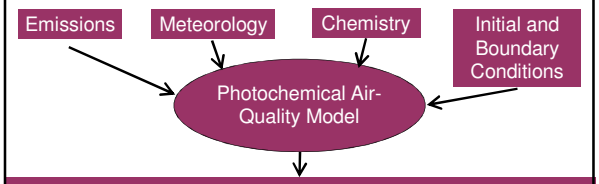


- $RRF = \frac{Simulated\ Future\ Year\ Concentration}{Simulated\ Base\ Year Concentration}$
- RRFs are specie and location specific

Future Mass → Future Design Value

- Select the highest eight FRM $PM_{2.5}$ days per quarter for 2005-2007 and SANDWICH them
- Project each component specie for each day into the future (There is an app for that!)
- Add components to get the total mass for each day
- Find the 98th percentile for each year
- Average 98th percentiles for three years to get the future Design Values

Photochemical Models → RRF



Concentrations of ozone, particulate matter, and other pollutants

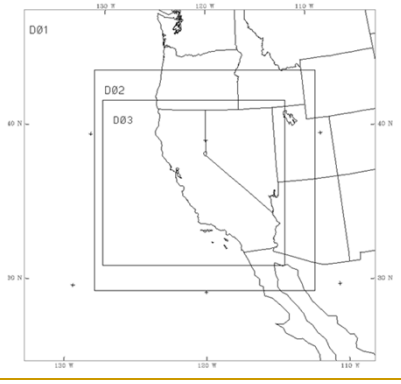
Models are mathematical representations of our best knowledge of atmospheric processes

Meteorology Modeling

- Modeling is conducted on a grid system
- A meteorology model is needed to provide meteorological parameters in each grid cell
- We use prognostic meteorology models (MM5 and WRF model) to generate 2007
- A coupled set of differential equations describing gradients in meteorological parameters solved
- NARR provides global-scale input
- 30 vertical layers up to 100 mb

MM5 – Mesoscale Model 5, WRF – Weather Research Forecast, NARR – North American Regional Reanalysis

Meteorology Domains

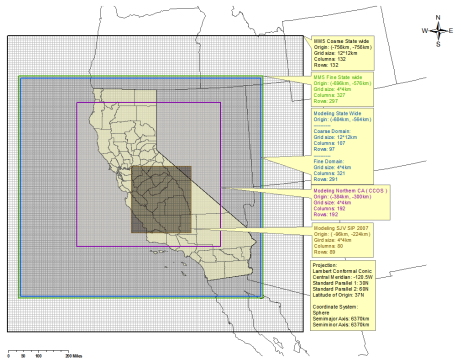


Air-Quality Modeling

- US EPA's CMAQ model
- SAPRC-97 chemistry
- Solves coupled sets of differential equations for advection, diffusion, and chemistry
- MOZART global model provides Initial and boundary conditions
- 15 vertical layers up to 100 mb

CMAQ – Community Multi-scale Air Quality
SAPRC – Statewide Air Pollution Research Center
MOZART – Model of Ozone and Related Trace Species

Air-Quality Domains



Model Performance Evaluation

- Operational (quantitative) – Ability to reproduce observed temporal and spatial patterns for meteorological parameters and pollutants
- phenomenological (qualitative) – General comparisons of observed features
- Diagnostic (semi-quantitative) – How accurate is the model in characterizing the sensitivity of $PM_{2.5}$ (and species) to changes in emissions?
- Corroborative (qualitative) – Model consistent with other analyses?

Limiting Precursors and Efficacies

- Precursors of interest are primary $PM_{2.5}$, NO_x, SO_x, VOC, and NH_3
- Last SIP simulations for the annual standard indicated that primary $PM_{2.5}$ and NO_x to be the most limiting precursors (in that order)
- Precursor equivalencies will be calculated based on current 24-hr SIP modeling
  - Can be thought of as "trading ratios" for precursors based on their effect on Design Values

Resource Requirements

- "Super" computer systems – Clustered PCs and workstations
- Highly technical staff with extensive training in mathematical modeling

The Core Modeling Team

- Project Lead:
  - Ajith Kaduwela – Ph.D. in Chemical Physics
- Meteorology Modeling:
  - Daniel Chau – Ph.D. in Civil and Environmental Engineering
  - Kemal Gürer – Ph.D. in Atmospheric Sciences
  - Zhao Zhan – Ph.D. in Atmospheric Sciences
- Air-Quality Modeling:
  - Jin Lu – Ph.D. in Chemical Engineering
  - Jeremy Avise – Ph.D. in Civil and Environmental Engineering
  - James Chen – Ph.D. in Earth Sciences/Engineering

The Modeling Support Team

Managers
- Sylvia Zulawnick
- Vernon Hughes
- Gabe Ruiz
- Steve Zelinka
- Mena Shah
- Pingkuan Di, Ph.D.

Emissions Inventory
- Kevin Eslinger
- Janet Spencer
- Charanya Varadarajan, Ph.D.

Emissions Forecasting
- Martin Johnson
- Adrian Griffin, Ph.D.

Emissions Gridding
- Cheryl Taylor
- Leo Ramirez, Ph.D.
- Wenli Yang, Ph.D.
- Anne Lin
- Don Johnson

Air Quality Analysis
- Patricia Velasco, Ph.D.
- Kasia Turkiewicz
- Jin Xu, Ph.D.
- Eugene Kim, Ph.D.
- Larry Larsen

Met Analysis
- Adam Gerber
- Elena Hanrahan

Current Status

- Emission gridding complete. QA/QC in progress.
- Meteorology modeling complete. Model performance analyses in progress.
- Air-Quality modeling in progress.
- Results to be presented in the summer.

Photochemical modeling is part of the Weight of Evidence that determines the attainment status.

Thank you very much for your attention!