Environmental
Programs

Technical Highlights of EPA's 7th Conference on Air Quality Modeling

Workshop Guide

APTI Workshop T-029

DAY 2

Developed by Environmental Programs - North Carolina State University
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Fax Question Sheet

APTI Workshop T-029

Technical Highlights of EPA's 7th Conference on Air Quality Modeling DAY 2

August 2, 2000

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Please write your question and direct it to the appropriate presenter if possible.

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APTI Workshop T-029

Technical Highlights of EPA's 7th Conference on Air Quality Modeling

Presented by OAQPS

Broadcast Agenda

August 2, 2000 1:00pm ET DAY 2

SECTION		TOPIC
1		Introduction *Jim Dicke*
2		**Alternative Models** ADMS *David Carruthers, Ph.D.* CAMx *Ralph Morris* SCIPUFF *Ian Sykes*
	10 MIN.	**BREAK**
3		**Alternative Models** HYROAD Introduction *Edward Carr* HYROAD Intersection Model *Robert Ireson* UAM-V *Edward Carr*
4		**Summary** *Joe Tikvart*
	10 MIN.	**BREAK**
		Questions and Answers and Wrap up

Technical Highlights of EPA's 7th Conference on Air Quality Modeling
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ADMS
Atmospheric Dispersion Modelling System

Dr. David J Carruthers
Cambridge Environmental
Research Consultants

ADMS

- Development commissioned in 1988 following a CERC report to regulatory authorities in the UK
- The CERC report highlighted the advantages of the use of surface/boundary layer scaling over Pasquill Gifford stability categories

ADMS

- Sponsors include UK's Environment Agency, UK Health and Safety Executive, major power and chemical companies

ADMS

- Development by:
  - CERC
    (including Prof. Julian Hunt,
    Dr. David Carruthers, Dr. Christine
    McHugh, Dr. Rex Britter)
  - University of Surrey
    (Prof. Alan Robins)
  - UK Meteorological Office
    (Dr. David Thomson)

ADMS

- ADMS is the leading European Short Range Air Dispersion Model and is used extensively in the UK and across Europe
- ADMS has featured in all 6 European Workshops on Harmonisation of Dispersion Models (1991-present)

Key Features of ADMS

- Continuous or discrete releases
- Point, line, area, volume and jet sources
  - treatment depends on receptor location

Key Features of ADMS

- Skewed-Gaussian model using local boundary layer variables
- Meteorological preprocessor
- Integral plume rise model

Key Features of ADMS

- Building effects
- Complex terrain
- Coastline
- Wet and dry deposition
- Chemical transformation

Key Features of ADMS

- Radioactive decay & gamma dose
- Jets and directional releases
- Concentration fluctuations module
- Condensed plume visibility module

Regulatory Applications

- Multiple buoyant or passive industrial emissions
- Surface, near surface or elevated releases
- Urban or rural areas
- Short (seconds) to long (annual) term averaging times

Flat Terrain Validation

Summary Scores for ISC3, ADMS and AERMOD (Different model input parameters)

Table 1

	ISC3	ADMS	AERMOD
Best	5	19	6
Middle	2	5	11
Worst	17	0	7

Table 2

	ISC3	ADMS	AERMOD
Best	4	8	10
Middle	10	15	11
Worst	10	1	3

Table 1 from Hanna et al, 6th Workshop on Harmonisation, France Oct 1999
Table 2 from Hanna et al, AWMA Meeting, US, June 2000

Power Station Comparison

Typical input data

Stack height (m)	200
Stack diameter (m)	13
Exit velocity (m/s)	22
Temperature (°C)	130
SO_2 emission rate (g/s)	5000

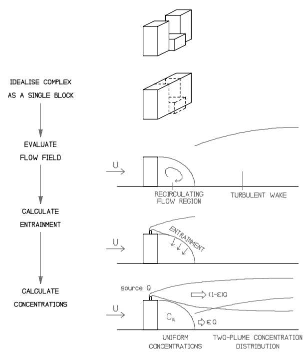
Meteorological data:

1 year of hourly sequential data from Manchester, UK, 1995

Maximum values of Percentiles and Annual Mean Concentration

	ADMS 3	AERMOD
100th	398	681
99.99th	310	669
99.9th	188	521
99th	97	180
98th	51	127
95th	3.9	54
90th	0.2	3.2
Annual mean	2.6	7.5

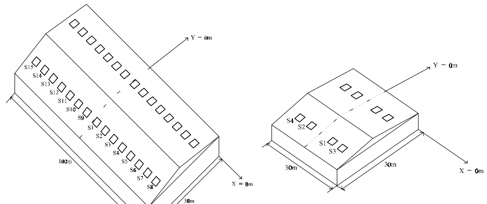
Modelling Building Effects



Two plume model

Based on flow field

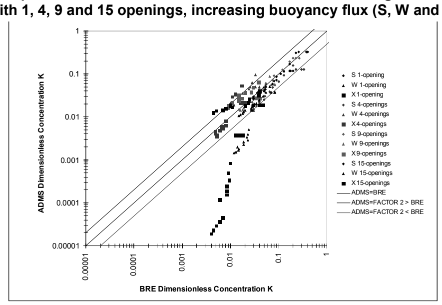
Building Validation - Wind Tunnel Experiment



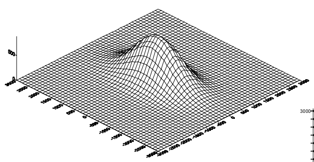
large building **small building**

Building Validation - Results

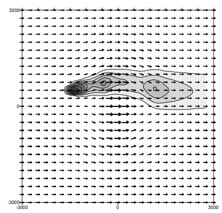
Comparison of ADMS with wind tunnel results for the large building with 1, 4, 9 and 15 openings, increasing buoyancy flux (S, W and X)



Complex Terrain Effects



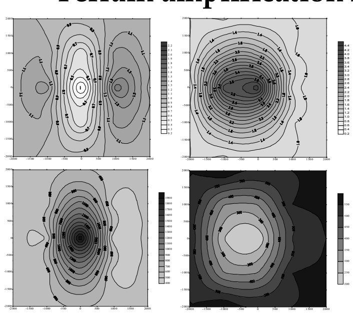
Based on modelled flow field



Above: View of idealized hill

Right: Flow field at 80m above terrain and ground level concentration from an 80m stack

ADMS and AERMOD Comparison: Terrain amplification factors



Left: ADMS Cmax
Right: AERMOD Cmax

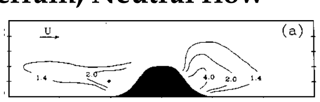
Ratio of complex terrain to flat terrain as function of stack location

- Neutral conditions
- 50m stack
- Idealised hill

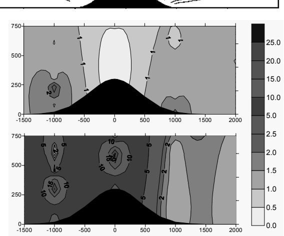
Left: ADMS Xmax
Right: AERMOD Xmax

ADMS and AERMOD Comparison: Complex terrain, Neutral flow

Wind tunnel, from Lawson et al



ADMS



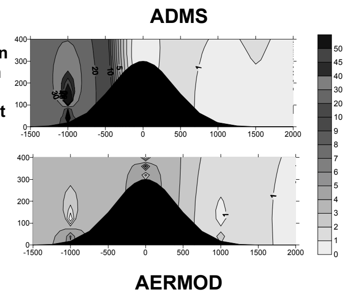
Ratio of complex terrain to flat terrain maximum concentrations as function of stack height and location

AERMOD

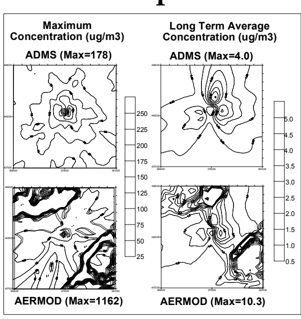
ADMS and AERMOD Comparison: Complex terrain, Stable flow

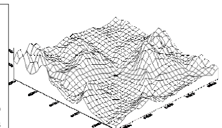
Ratio of complex terrain to flat terrain maximum concentrations as function of stack height and location

- Wind Speed (10m) = 0.76 m/s
- Monin-Obukhov length = 23 m



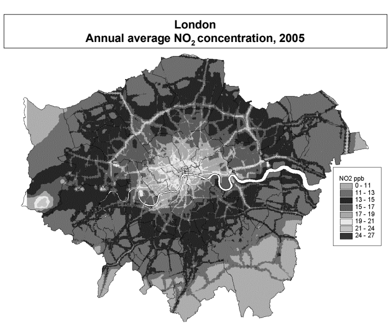
ADMS and AERMOD Comparison: Complex terrain results





Stack and surrounding terrain

ADMS-Urban



- Advanced air quality model for major cities and airports
- Includes algorithms for dispersion from roads and street canyons
- Used in major cities in Europe and beyond

Summary

- ADMS includes in one model all the features of AERMOD (except input of observed boundary layer profiles), ISC-PRIME and CTDM PLUS – potential difficulties arising as to whether to use AERMOD or ISC-PRIME avoided (e,.g, at site with buildings and tall stacks)

Summary

- Additionally ADMS includes concentration fluctuation, plume chemistry and condensed plume visibility algorithms

Summary

- ADMS-Urban includes capabilities of CALINE, most features of EDMS and other features
- The costs of ADMS are similar to commercially available versions of AERMOD and ISC

Summary

- ADMS was first released in 1993 and has been used in many critical applications
- There are over 500 licenses worldwide

http://www.cerc.co.uk

Comprehensive Air-quality Model with extensions (CAMx)

Ralph E. Morris
ENVIRON International Corp.

CAMx Version 2.00

- 3-D Eulerian tropospheric photochemical transport model
  - treats emissions, chemistry, dispersion, removal of gaseous and aerosol air pollution
  - scales range from individual point sources (< 1 km) to regional (>1000 km)

CAMx Version 2.00

- Combines features required of "state-of-the-science" models
  - new coding of several industry-accepted algorithms
  - computationally and memory efficient
  - easy to use

CAMx Version 2.00

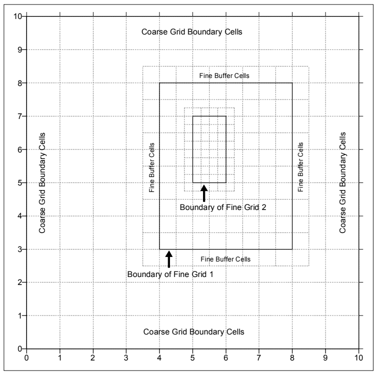
- modular framework permits easy substitution of revised and/or alternate algorithms
- publicly available (www.camx.com)

CAMx Version 2.00

- Technical Features:
- Grid nesting
  - two-way horizontal and vertical nesting
  - supports multiple levels
  - variable meshing factors

CAMx Version 2.00

- Plume-in-Grid (PiG) sub-model
- Multiple, fast and accurate chemical mechanisms
- Mass conservative and mass consistent transport scheme



CAMx Version 2.00

- Multiple map projections
  - curvi-linear latitude/longitude
  - Universal Transverse Mercator
  - Lambert Conformal (MM5)
  - Rotated Polar Stereographic (RAMS)

CAMx Version 2.00

- Ozone Source Apportionment (OSAT)
  - tracks source region/category contributions to receptor ozone concentrations
  - indicates if ozone formed in NO_x or VOC-limited conditions

CAMx Version 2.00

- Ability to use historical air quality model databases developed for other models
  - OTAG, LMOS, COAST/Houston, Atlanta, Northeast Corridor

Key Technical Components

- Overview
  - solves continuity equation for each species
  - time splitting operation
    - each process solved individually for each grid, each time step
  - time step size maintains stable solution of transport on each grid

Key Technical Components

- multiple transport steps per master grid step required for
- nested grids
- multiple chemistry steps per transport step required
- model developed to run on meteorological modeling grid
  - reduces error due to interpolation and averaging
  - multiple map projections available

Key Technical Components

- Transport
  - advection and diffusion solvers are mass conservative
  - horizontal and vertical advection linked through the divergent compressible atmospheric continuity equation
    - mass consistency

Key Technical Components

- order of east-west and north-south advection alternates each master grid step
- three options available for horizontal advection solvers:
  - Smolarkiewicz (1983): diffusion-corrective forward-upstream scheme
  - Bott (1989): area-preserving flux-form solver
  - Piecewise Parabolic Method (PPM)

Key Technical Components

- Transport (concluded)
  - vertical transport and diffusion solved with an implicit scheme
  - dry deposition rates are used as the surface boundary condition
  - horizontal diffusion solved with an explicit scheme in two directions simultaneously

Key Technical Components

- Pollutant Removal
  - dry deposition velocities for each species determined using resistance approach (Wesely, 1989)
    - dependent upon: season, land cover, solar flux, near-surface stability, surface wetness, species solubility and diffusivity
    - for aerosols: size spectrum dictates sedimentation velocity

Key Technical Components

- wet scavenging based on Maul (1980) as implemented in CALPUFF (EPA, 1995)
  - exponential decay
  - decay rate dependent upon: rainfall rate, species solubility
  - species removed from entire grid column (all layers)

Key Technical Components

- Photochemistry
  - CBM-IV (Gery et al., 1989)
    - 3 variations available
  - SAPRC97 (Carter, 1990)
    - chemically up-to-date
    - tested extensively against environmental chamber data
    - uses a different approach for VOC lumping

Key Technical Components

- all mechanisms are balanced for nitrogen conservation
- photolysis rates derived from TUV preprocessor
  - generates lookup table over: zenith angle, altitude, ozone column, albedo, turbidity
  - first two determined for each grid cell internally
  - last three provided by input files

Key Technical Components

- photolysis rates affected by clouds
  - UAM-V approach: rates scaled by fractional cloud coverage only
  - RADM approach: rates scaled by optical depth and cloud coverage

Key Technical Components

- Chemistry Solver
  - most "expensive" component of photochemical grid simulations
  - CAMx solver increases efficiency and flexibility
  - adaptive hybrid approach:
    - radicals (fastest reacting species) solved using implicit steady state approximation

Key Technical Components

- fast state species solved using second-order Runge-Kutta method
- slow state species solved explicitly
- "Adaptive" = number of fast state species changes according to the chemical regime

Key Technical Components

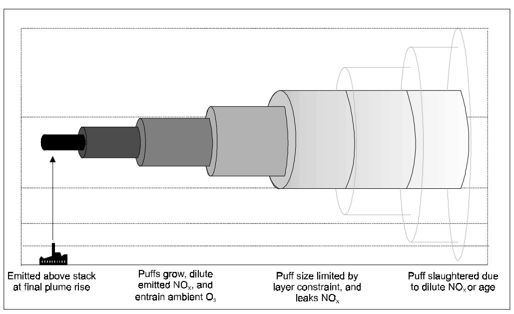
- Plume-in-Grid (PiG)
  - fine resolution needed for near-source chemistry/dispersion of large NO_x plumes
  - tracks stream of plume segments (puffs) in a Lagrangian frame
    - each puff moved by winds in host cell
    - puff growth (dispersion) determined by diffusion coefficients in host cell

Key Technical Components

- GREASD PiG: faster, conceptually simpler
  - reduced NO_x chemistry set (NO-NO, NO_x/ozone equilibrium, HNO_3 production)
  - cross-sectional Gaussian pollutant distribution

Key Technical Components

- puffs leak mass according to growth rates and grid cell size
- puffs terminated due to age or sufficiently dilute NO_x



Key Technical Components

- Ozone Source Apportionment (OSAT)
  - determines source area/category contributions to ozone anywhere in the domain
  - uses tracers to track precursor emissions and ozone production/destruction

Key Technical Components

- also tracks contribution of initial and boundary conditions
- estimates whether ozone is produced under NO_x- or VOC-limited conditions

Key Technical Components

- removes need to run model repeatedly to understand:
  - chemical regime
  - influences of various sources
- HOWEVER: cannot quantify ozone response to NO_x or VOC controls

Key Technical Components

- CAMx Version 2.00 PM Treatment
  - Primary Particulate Matter (PM)
  - Secondary Organic Aerosols (SOA) treated using aerosol yield approach in photochemistry
  - Sulfate/Nitrate/Ammonia equilibrium aerosol thermodynamics using empirical UAM/LC approach
  - Empirical aqueos-phase (Sulfate)

CAMx Version 3 Attributes Coming Summer 2000 (www.camx.com)

- Flexi-nesting
  - Ability to add/delete nested-grids during a simulation
  - Real time interpolation of fine-grid inputs from next coarser grid

CAMx Version 3 Attributes Coming Summer 2000 (www.camx.com)

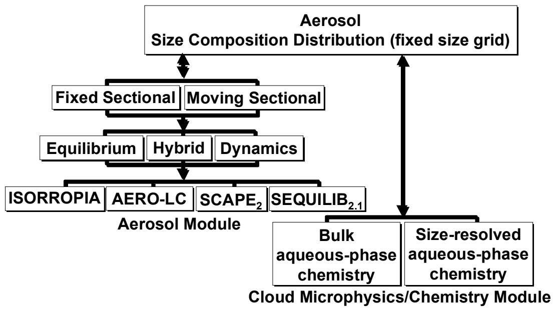
- Decoupled Direct Method (DDM)
  - Sensitivity coefficients provides information on the relationship of CAMx-estimated ozone (or other species) and sources of precursors (emissions, boundary conditions, and initial concentrations)

CAMx Version 3 Attributes Coming Summer 2000 (www.camx.com)

- Information is useful for
  - Control Strategy Development
  - Model performance evaluation
  - Diagnostic analysis

CAMx Version 3 Attributes

Advanced PM Treatment



CAMx Version 3 Attributes

Advanced PM Treatment

Gas-Phase Chemistry:	1) SAPRC97 2) Enhanced CBM-IV (monoterpines)
Size Section:	1) Fixed Section 2) Moving Section
Mass Transfer:	1) Equilibrium 2) Hybrid 3) Dynamic

CAMx Version 3 Attributes

Advanced PM Treatment

Aerosol Thermo-dynamic:	1) LCAERO (parameterized RFM) 2) SCAPE2 (full science) 3) ISORRPIA (significantly faster)
Aqueous-Phase Chemistry:	1) Bulk 2) Size Resolved 3) Empirical (existing)
Secondary Organic Aerosol:	1) SOAM2 2) Aerosol Yields (existing)

CAMx Version 3 Attributes

Advanced PM Treatment

Coagulation:	1) CMU algorithm
Nucleation:	1) CMU algorithm
Dry Deposition:	1) Wesley gaseous (existing) 2) AERO particle dry deposition
Wet Deposition:	1) Rainout and washout as part of aqueous-phase module 2) Existing gaseous wet deposition interface with aqueous-phase module

CAMx Postprocessing and Analysis Tools

- CAMxtrct
  - Extracts and reformats CAMx output for multiple grids (Fortran)
- SURFER (by Golden Software)
  - Visualization (PC based)

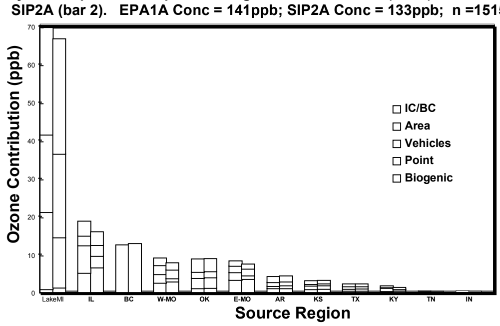
CAMx Postprocessing and Analysis Tools

- MAPS (by Alpine Geophysics)
  - Model evaluation and visualization (Fortran/NCAR graphics)
- PAVE (by MCNC)
  - Visualization (Unix/LINUX)

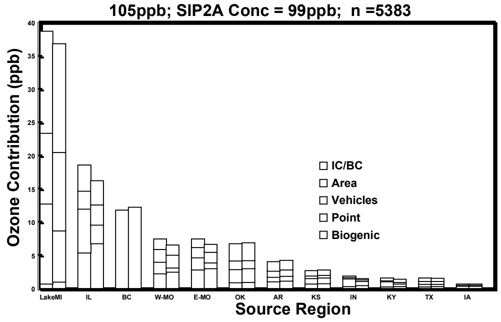
CAMx Postprocessing and Analysis Tools

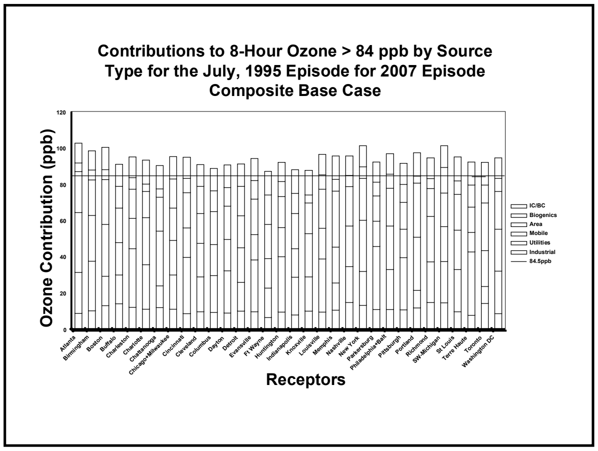
- VIS5D
  - Visualization (various)
- CAMxDESK (by EnviroModeling)
  - Visualization and analysis software (PC based)

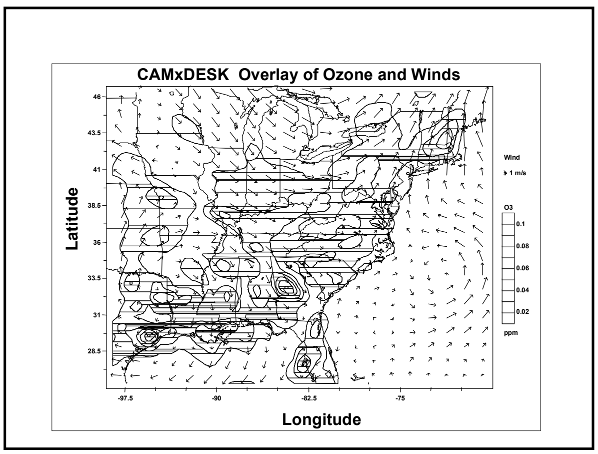
Contribution to 1-Hour Ozone > 124ppb in the Lake Michigan Region for the July, 1995 Episode Composite using Base Case EPA1A (bar 1) and SIP Call SIP2A (bar 2). EPA1A Conc = 141ppb; SIP2A Conc = 133ppb; n =1515

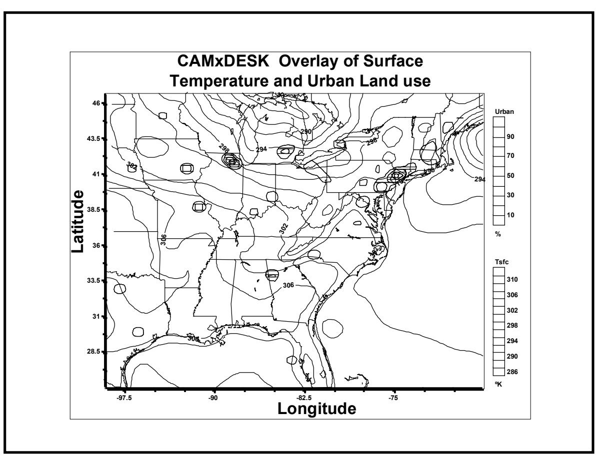


Contribution to 8-Hour Ozone > 84ppb in the Lake Michigan Region for the July, 1995 Episode Composite using Base Case EPA1A (bar 1) and SIP Call SIP2A (bar 2). EPA1A Conc = 105ppb; SIP2A Conc = 99ppb; n =5383




Contributions to 8-Hour Ozone > 84 ppb by Source Type for the July, 1995 Episode for 2007 Episode Composite Base Case
Ozone Contribution (ppb)
0
20
40
60
80
100
120
Atlanta
Birmingham
Boston
Buffalo
Charleston
Charlotte
Chattanooga
Chicago+Milwaukee
Cincinnati
Cleveland
Columbus
Dayton
Detroit
Evansville
Ft Wayne
Huntington
Indianapolis
Knoxville
Louisville
Memphis
Nashville
New York
Parkersburg
Philadelphia+Balt
Pittsburgh
Portland
Richmond
SW-Michigan
St Louis
Terre Haute
Toronto
Washington DC
Receptors
IC/BC
Biogenics
Area
Mobile
Utilities
Industrial
84.5ppb


CAMxDESK Overlay of Ozone and Winds
Latitude
Longitude
Wind
1 m/s
O3
0.1
0.08
0.06
0.04
0.02
ppm


CAMxDESK Overlay of Surface Temperature and Urban Land use
Latitude
Longitude
Urban
90
70
50
30
10
%
Tsfc
310
306
302
298
294
290
286
°K

Second-order Closure Integrated Puff (SCIPUFF)

R. Ian Sykes
ARAP Group
Titan Corporation

Overview

- Modeling Approach
- Graphical User Interface
- Input/Output
- Model Evaluation Studies

Lagrangian Puff Model

- Concentration field - collection of overlapping puffs with Gaussian distributions
- Concentration given by sum over all puffs
- Solve ODE's for puff moments

Lagrangian Puff Attributes

- **Arbitrary range of scales without numerical grid and associated diffusion errors**
- **Arbitrary time-dependent, spatially inhomogeneous conditions**
- **Multiple sources with arbitrary time-dependence**

Concentration Field

$$c(x) = \sum_{\alpha} c^{(\alpha)}(x) = \sum_{\alpha} Q^{(\alpha)} G^{(\alpha)}(x)$$

where

$$G^{(\alpha)} = \frac{1}{V} \exp\left[-\frac{1}{2} \left(\sigma_{ij}^{(\alpha)} \right)^{-1} \left(x_i - \bar{x}_i^{(\alpha)} \right) \left(x_j - \bar{x}_j^{(\alpha)} \right) \right]$$

$Q^{(\alpha)} =$ total mass of puff (zeroth moment)

$\bar{x}_i^{(\alpha)} =$ puff centroid (first moment)

$\sigma_{ij}^{(\alpha)} =$ spatial spread (second moment)

$V =$ puff volume $= (2\pi)^{3/2} \left\| \sigma^{(\alpha)} \right\|^{1/2}$

Puff Moment Equations

$$\frac{d}{dt} Q^{(\alpha)} = 0$$

$$\frac{d}{dt} \bar{x}_i^{(\alpha)} = \bar{u}_i\left(\bar{x}^{(\alpha)}, t\right)$$

$$\frac{d}{dt} \sigma_{ij}^{(\alpha)} = \frac{\left\langle \overline{x_i' u_j' c'} \right\rangle^{(\alpha)} + \left\langle \overline{x_j' u_i' c'} \right\rangle^{(\alpha)}}{Q^{(\alpha)}} + \sigma_{ik}^{(\alpha)} \partial \bar{u}_j + \sigma_{jk}^{(\alpha)} \partial \bar{u}_i$$

Turbulence Closure

$$\frac{d}{dt}\left\langle x_i' \overline{u_j' c'} \right\rangle^{(\alpha)} = Q^{(\alpha)} \overline{u_i' u_j'} - \frac{Aq}{\Lambda} \left\langle x_i' \overline{u_j' c'} \right\rangle^{(\alpha)}$$

where $q^2 = \overline{u_i' u_i'}$ and Λ is the turbulence length scale.

Turbulent Dispersion

- **Closure model gives direct relationship between turbulence quantities and diffusion rates**
- **Provides single diffusion model framework for a wide range of atmospheric scales**

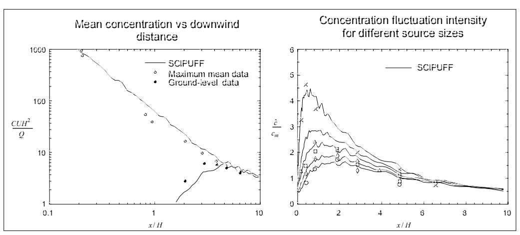
Model Efficiency

- **Puff splitting allows accurate treatment of wind shear**
- **Puff merging minimizes number of puffs**
- **Efficient adaptive time-step algorithm**
- **"Static" puffs for steady-state section of plume**

Concentration Fluctuations

- Turbulent dispersion implies a random concentration field
- 2nd-order closure model gives both fluctuation variance, $\overline{c'^2}$, and $\overline{c}$
- The probability distribution of c is then modeled by the clipped normal distribution

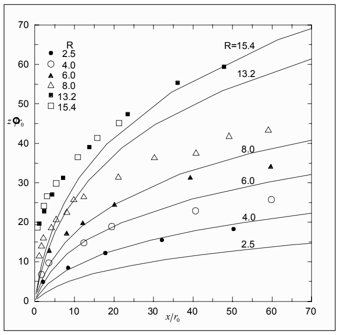
Fackrell & Robins (1982)



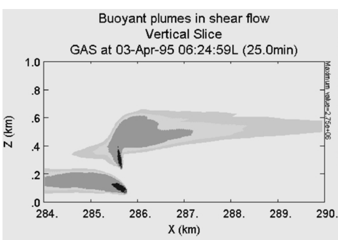
Plume Rise

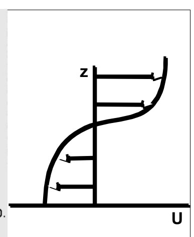
- Associate dynamic vertical momentum and temperature perturbation integrals with each puff
- Add evolution equations for puff dynamics based on conservation of momentum and temperature

Momentum Rise



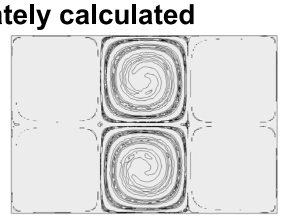
Buoyant Rise





Wind Shear

- Use complete (six-moment) Gaussian specification so that shear distortions can be accurately calculated



Model Input

- Source Data
  - Pollutant physical and chemical properties
  - Release type

Model Input

- Meteorological Data
  - Fixed winds
  - Observational Input (surface and/or profile)
  - Time-dependent 3-dimensional gridded

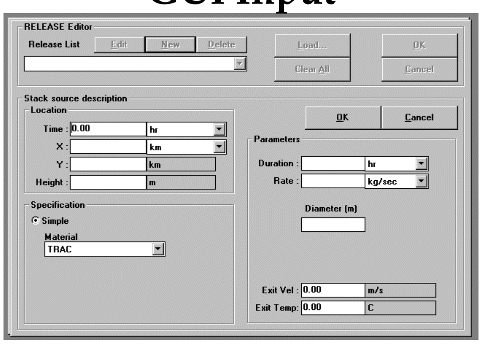
Model Input

- Terrain for mass consistent wind field
- Turbulence Data
  - Planetary boundary layer
  - Large scale variability

Model Input

- Boundary layer turbulence
  - Profiles based on wind speed, roughness, and surface heat flux calculation

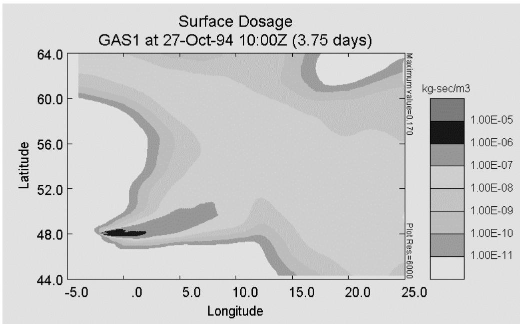
GUI Input



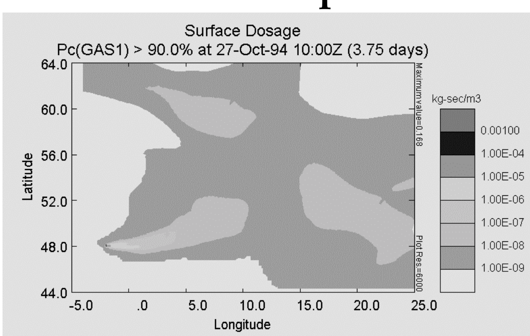
Model Output

- Sampler file
  - Time history at receptor locations
- GUI plots
  - Horizontal slices
  - Vertical slices
  - Integrated surface deposition and dose
  - Probability

GUI Output



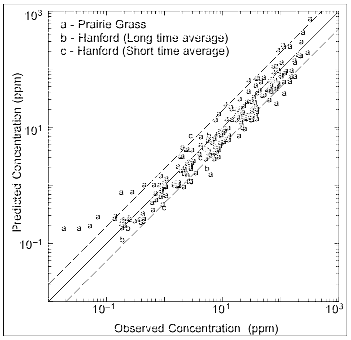
GUI Output



Model Evaluation Studies

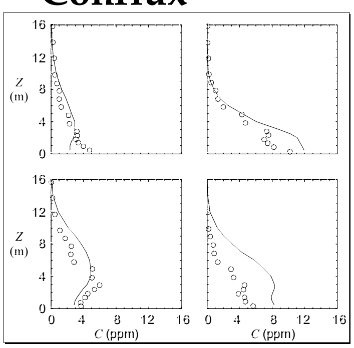
- **PGT curves**
- **Instantaneous dispersion data**
- **Lab dispersion and fluctuation data**
- **Continental-scale ANATEX field experiment**
- **EPRI PMV&D tall-stack emissions**
- **CONFLUX (short range, fluctuations)**
- **Dugway field tests**
- **Model Data Archive**
- **ETEX**

MDA Passive



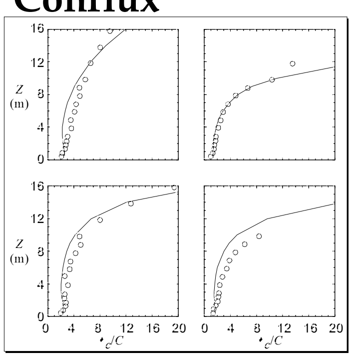
Conflux

Mean Concentration

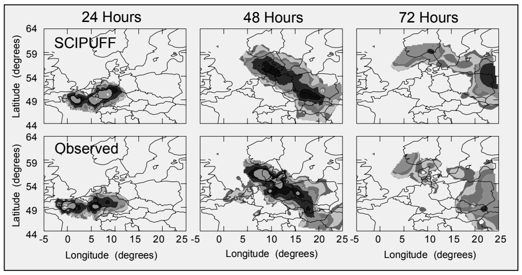


Conflux

Concentration Fluctuation Intensity



ETEX



Model Availability

Available for downloading from the Titan website: www.titan.com/systems/prod.htm

The Hybrid Roadway Intersection Model: HYROAD

Edward Carr and
Robert Ireson
ICF Consulting

Contact Information

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Overview

- Background
- Scientific basis and model formulation
- Model application - resource needs

Overview

- Model sensitivity and performance
- Proposed applications
- Project status and next steps

Background

- SIP, conformity, and EIS "Hot-Spot" analysis for carbon monoxide (CO)
- Sponsorship: NCHRP, FHWA

Background

- Four phase study:
  - Problem assessment - Site Monitoring Plan (1993-1995)
  - Site monitoring and evaluation - Data Collection & Analysis (1993-1997)
  - Model development - Evaluation & Testing (1997-2000)
  - Development GUI & user guide (2000-2001)

Primary Objectives of Research

- Assemble a comprehensive national database
  - Model testing and evaluation

Primary Objectives of Research

- Developed an improved fully integrated roadway intersection model
  - Dispersion
  - Emissions
  - Traffic

Approach to Model Development

- Analysis of field program data to characterize dynamic processes
  - Assess those elements most important and incorporate into model framework
- Develop model based on understanding of key processes

Scientific Basis and Model Formulation

- Intersection model components
- Limitations of existing models
- Field study design and findings
- HYROAD formulation

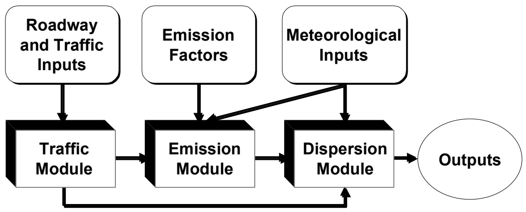
Intersection Dynamics

- Traffic
  - Queuing
  - Acceleration, deceleration, and cruise
  - Non-steady state

Intersection Dynamics

- Emissions and dispersion
  - Modal effects (e.g., power enrichment)
  - Buoyancy and vehicle wake turbulence
  - Short transport distances

Intersection Model Components



The need for integration

Limitations of Existing Models

- CAL3QHC simplifications
  - Two emission states -- idle or cruise
  - Steady state meteorology (PG sigma-y and sigma-z)
  - Queuing based on quality of progression

Limitations of Existing Models

- CALINE4 approaches
  - Empirical emission adjustment for acceleration
  - Roadway turbulence and buoyancy
  - Use of sigma-theta in place of sigma-y

Field Study Elements - Continuous

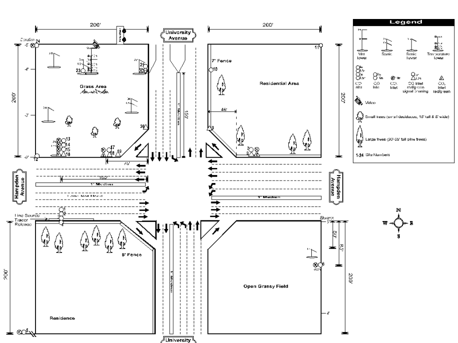
(15 minute average)

- Traffic approach volume and signal timing
- Meteorology
  - 3 m and 10 m wind speed and direction
  - Temperature, RH, sigma-theta, stability

Field Study Elements - Continuous

(15 minute average)

- CO and CO_2 at 16+ locations
- Sonic anemometers (2- and 3-axis)



Field Study Layout

Field Study Elements -- Short-term Studies

- Floating car runs
  - Time-distance data (1 second resolution)
- Coldstart survey (distance from trip origin)

Field Study Elements -- Short-term Studies

- Tracer study (SF6)
  - Light wind periods
  - 15-minute averages at multiple receptors

Field Study Findings -- Flows and Turbulence

- Induced flows of 3+ m/s at roadside
- Induced flows and enhanced turbulence observable at >25 m from roadside

Field Study Findings -- Flows and Turbulence

- Observed vertical dispersion rate exceeds both PG and CALINE3/CAL3QHC
- SF6 tracer observed >100 m 'upwind' of release point due to induced flows

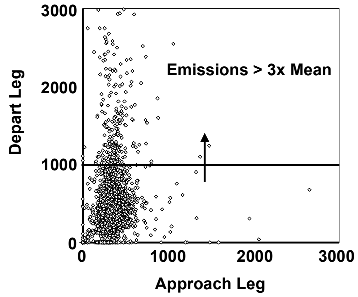
Field Study Findings -- Traffic and Emissions

- Speed/acceleration distributions do not resemble any emission test cycles
- Power enrichment occurs on depart legs

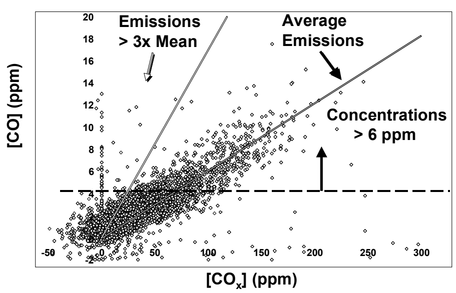
Field Study Findings -- Traffic and Emissions

- Constant g/gal emission rates observed at all locations for high concentration periods
- Enrichment does NOT appreciably contribute to high concentrations

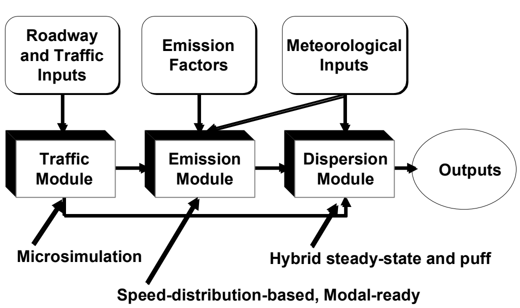
Emissions (g/gal) Show Enrichment on Acceleration



High CO Events Show Little Enrichment



HYROAD Formulation



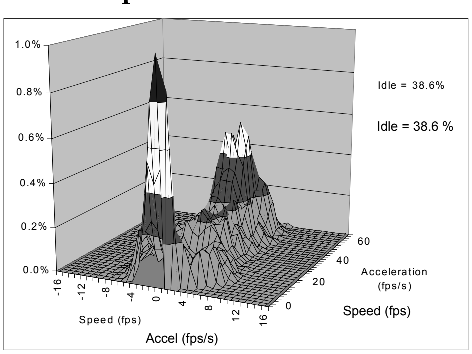
Traffic Module - Micro-simulation

- Based on TRAF-NETSIM - simulation of vehicle movements at 1 second resolution
- Explicit treatment of traffic patterns
  - Turn lanes, signal phases, queuing
  - Coordination of upstream signals

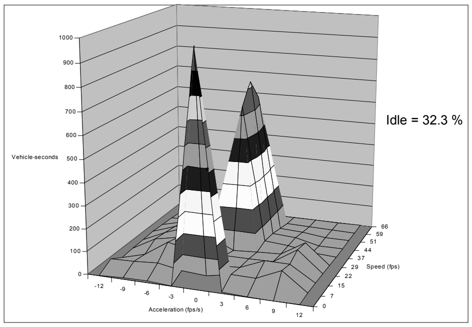
Traffic Module - Micro-simulation

- Output: Speed/acceleration distribution by 10 m roadway segment and signal phase

Denver Speed-Acceleration Profile



HYROAD Speed-Acceleration Profile (LOS C Test Case)



Emission Module

- Objective: make the best possible use of cycle-based emission factors
- Core rates from MOBILE5 for the speeds of the speed correction cycles

Emission Module

- Multivariate regression weights speed correction cycles to match non-idle speed distribution from NETSIM

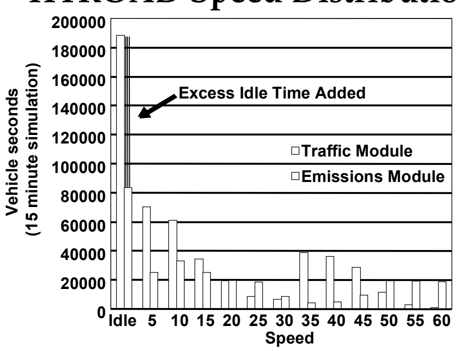
Emission Module

- Total emissions calculated from weighted average g/mi rate plus excess idle (idle time not explained by weighted cycles)
- Speed/acceleration distributions used to calculate fuel consumption by 10 m roadway segment and signal phase

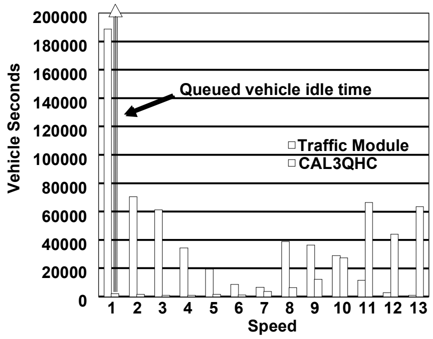
Emission Module

- Fuel consumption used as a surrogate to spatially and temporally allocate emissions

HYROAD Speed Distribution



CAL3QHC Speed Distribution



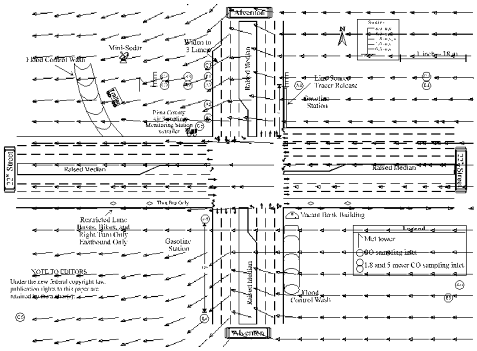
Induced Turbulence and Flow Fields

- Based on ROADWAY (Eskridge, 1987)
- Turbulence and induced flow calculated for each 10 m roadway segment using traffic volume and speed

Induced Turbulence and Flow Fields

- Output for each signal phase: Gridded wind speed and eddy diffusivity for a 2.5 x 2.5 km grid of 10 m cells

Wind Field with Induced Flows



Dispersion Module

- Gaussian model (moderate wind)
  - Uses CALINE4 mixing zone, sigma-z, sigma-theta
- Puff model
  - 1 puff per second per 10 m roadway segment
  - Puff transport with gridded winds by phase

Dispersion Module

- Puff growth based on local stability from gridded eddy diffusivity
- Domain wind and stability used after 1 cycle

Model Formulation - Conclusions

- HYROAD integrates accepted modeling approaches to treat important processes affecting intersection CO concentrations
  - Induced flows and turbulence
  - High spatial and temporal variability of emissions

Model Formulation - Conclusions

- Modular design allows updating (e.g., for modal emissions)

Model Application - Resource Needs

- Standard inputs
  - Intersection geometry (lanes, medians, etc.)
  - Traffic (volume, turns, signal cycles, speeds, coordination)

Model Application - Resource Needs

- Meteorology (wind speed, direction, stability, temperature, optional sigma-theta
- Emission factors by temperature (constant cold-start), or hour-specific

Model Application - Resource Needs

- Input preparation time
  - Geometry and NETSIM: 8 hours
  - Emissions and Dispersion: 12 hours

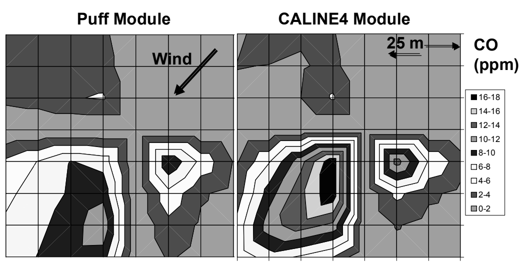
Model Application - Resource Needs

- Run time (500 MHz Pentium, 128 Mb)
  - Netsim: 30 sec / simulation hour
  - Dispersion: 4 min / simulation hour
  - Optimization possibilities

HYROAD Sensitivity and Performance

- Sensitivity analyses
  - Nominal intersection with grid of receptors in NW quadrant
  - Modeling with both Gaussian and puff models
  - Results for wind speed, wind direction, and stability

Concentration Patterns -- Puff v. CALINE4



HYROAD Sensitivity and Performance

- Performance evaluation data sets
  - Intensive data sets for three intersections
    - 528 hours with 15 minute data (6000 available)
    - 10 or more receptor locations

HYROAD Sensitivity and Performance

- 8 SLAMS/NAMS sites
  - 1728 hours (75,000 available)
  - Uncertain background concentrations

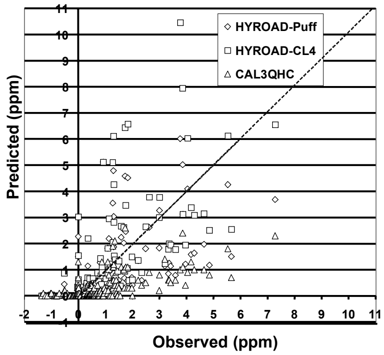
HYROAD Sensitivity and Performance

- Performance evaluation approach
  - Concurrent evaluation of HYROAD (Gaussian and puff) with CAL3QHC without regulatory constraints (D, 1 m/s)

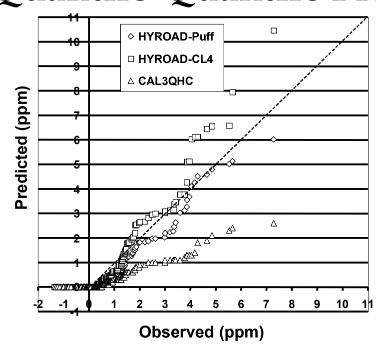
HYROAD Sensitivity and Performance

- Scatterplots, stratified by receptor, wind speed, and wind direction
- Standard statistics
  - All data
  - Max 25 paired
  - Max 25 unpaired

Predicted vs. Observed [CO]



Quantile-Quantile Plot



Preliminary Performance Results

- HYROAD produces more accurate robust high concentration than CAL3QHC
- Performance differences observed between receptor locations
- HYROAD appears to provide improved treatment of problematic worst-case conditions

Preliminary Performance Results

- Performance evaluation for other intersections is under way
- Screening methodology using HYROAD will be developed and evaluated

Proposed Applications

- Refined CO Applications
  - SIPs
  - Conformity
  - EIS/EIR
- Particulate matter "hot-spots" assessment
- Air toxic risk assessment

Project Status

- Current Status
  - Select transition from puff to line-segment
  - Complete model performance evaluation
    - Completed Tucson
    - Virginia & Denver plus 8 SLAMS/NAMS sites

Project Status

- Present Evaluation and Recommendations to NCHRP panel

Next Steps

- Develop Graphical User Interface
  - Facilitate communication between modules
  - Ease burden for user in developing inputs
- Update Draft User Guide
  - Reflect changes

Next Steps

- Schedule for Completion
  - Complete Evaluation (August 2000)
  - Develop GUI and Beta Testing (Fall 2000)
  - Update User Guide (Winter 2000-2001)

The Variable Grid Urban Airshed Model (UAM-V, UAM-VPM)

Edward Carr

Overview of the Variable-Grid Urban Airshed Model (UAM-V)

- Simulates the physical and chemical processes governing the formation and transport of ozone in the troposphere
  - three-dimensional, Eulerian (grid-based) model

Overview of the Variable-Grid Urban Airshed Model (UAM-V)

- requires specification of meteorological, emissions, land-use, and other geographic inputs
- output includes hourly concentrations of ozone and precursor pollutants for each grid cell within a (three-dimensional) modeling domain

Overview of UAM-V

- Core model, supporting software, user's manuals, and example modeling database available from SAI at no charge
- www.uamv.saintl.com

Overview of UAM-V

- Version 1.24 – OTAG version
  - Updated isoprene chemistry (1996)
- Version 1.30 – Latest version
  - Toxics chemistry, process analysis

UAM-V Modeling System Features

- Carbon-Bond-IV chemical mechanism with enhanced isoprene and toxics chemistry
- Two-way interactive nested-grid capabilities
- Plume-in-grid (P-i-G) treatment

UAM-V Modeling System Features

- Accepts output from a variety of dynamic meteorological models (e.g. MM5)
- Contains "process analysis" capabilities

Treatment of Processes in UAM-V

- Advective pollutant transport
  - Smolarkiewicz scheme
- Turbulent diffusion
  - Dispersion proportional to concentration gradient – K Theory

Treatment of Processes in UAM-V

- Surface removal
  - Uptake of pollutants by various surface features - land use
- Chemistry
  - Carbon Bond IV chemical mechanism with updated isoprene chemistry and toxics mechanism

UAM-V Modeling System

- Core model and input processing software
- Emissions Preprocessing System (EPS2.5) to prepare ozone and particulate emission inventories
- UAM-V Postprocessing System (UPS)

UAM-V Modeling System

- Process analysis modeling system software
- Model Output Visualization and Input Evaluation Software (MOVIES) – Color animations

UAM-V Input File Requirements

- Meteorological input files
  - wind
  - temperature
  - water-vapor concentration
  - pressure

UAM-V Input File Requirements

- vertical diffusivity (effective mixing height)
- cloud cover
- rainfall rate

UAM-V Input File Requirements

- Emissions input files
  - low-level anthropogenic emissions
    - point sources
    - area sources
    - motor-vehicles
  - elevated point source emissions
  - biogenic emission estimates

UAM-V Input File Requirements

- Air quality related input files
  - initial conditions
  - boundary conditions
- Chemistry input files
  - chemical reaction rates
  - photolysis rates

UAM-V Input File Requirements

- Geographic/other input files
  - land-use
  - albedo, turbidity, and ozone column

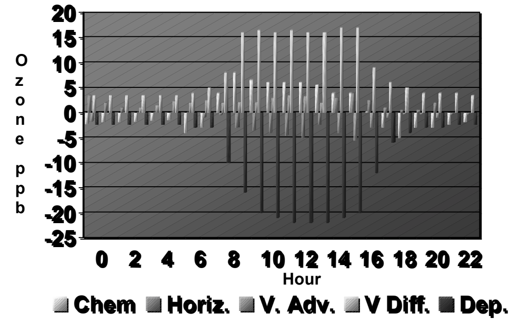
UAM-V Process Analysis Capabilities

- UAM-V process analysis provides detailed information on the physical and chemical simulation processes
- Process-level information includes
  - photochemical production/consumption

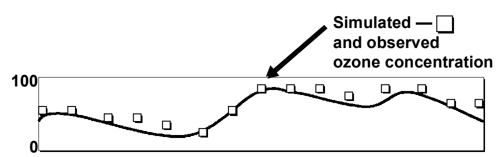
UAM-V Process Analysis Capabilities

  - horizontal advection/diffusion
  - vertical advection
  - vertical diffusion
  - deposition
  - emissions (for precursor pollutants)

Simulated Process Contributions to Ozone



Simulated Process Contributions to Ozone



UAM-V Users/Applications

- Over 60 registered users worldwide (Version 1.30), unknown number of unregistered users
  - U.S. EPA, state/local agencies, and industry
  - Environment Canada

UAM-V Users/Applications

- European research and regulatory agencies
- European and Japanese auto-makers; European oil companies

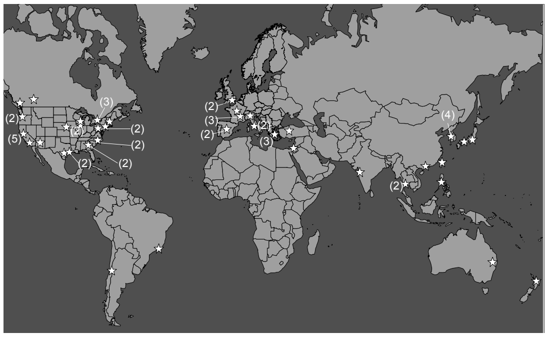
UAM-V Users/Applications

- Registered users
  - Research and regulatory groups in Central and South America, Australia, New Zealand, and several Asian countries including
    - China
    - Taiwan
    - South Korea
    - Philippines
    - India
    - Thailand (AIT)

UAM-V Users/Applications

- Some completed applications
  - Numerous U.S. regions/cities
    - OTAG, Atlanta, Houston, Baton Rouge, Chicago
  - Vancouver,B.C.
  - U.K.
  - Paris
  - Milan
  - Mexico City
  - Athens

Worldwide Users of the UAM-V Modeling System



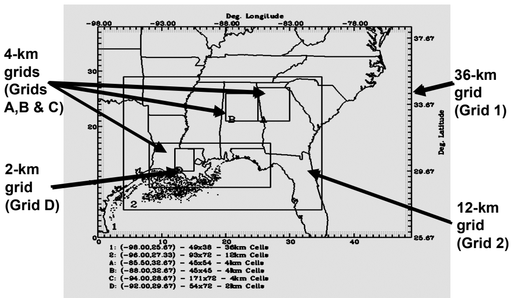
Current Applications

- Gulf Coast Ozone Study (GCOS) – Assessment of ozone formation and transport processes affecting 1- and 8-hour ozone along the U.S. Gulf Coast

Current Applications

- Arkansas-Tennessee-Mississippi Ozone Study (ATMOS) – Assessment of potential 8-hour ozone issues for Memphis, Nashville, Knoxville, Tupelo, Chattanooga, and Little Rock
- Mexico City - Demonstration for a new area/preliminary emissions sensitivity analysis

Example of a Multiple Nested Domain: Gulf Coast Ozone Study



Overview of the UAM-VPM

- UAM-V photochemical model (CB-2000)
- Particulate matter (PM) stand-alone box model employing hybrid modal-sectional approach to PM representation
- Gas-phase chemical mechanism generator for the UAM-V

Structure of the UAM-VPM

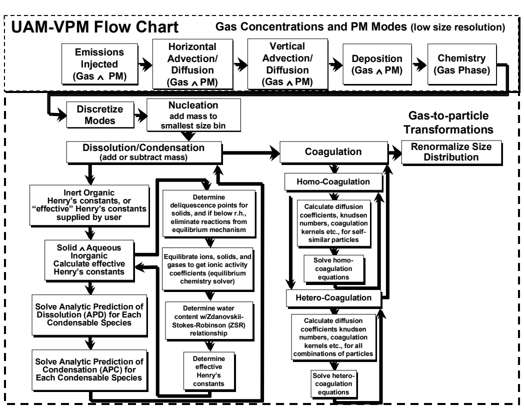
- Features of PM dynamics that can be well characterized by known algorithms are hard coded
- Features which are not well known are user inputs or dynamically selected
- Allows for the best research grade algorithms to be used in a regulatory and planning platform

PM Processes in UAM-VPM

1) Modal discretization (new)
2) Nucleation
(Fitzgerald, Hoppel, Gelbard, 1998)
3) Coagulation
(Jacobson, 1994, 1999)
4) Condensation
(Jacobson, 1997, 1999)

PM Processes in UAM-VPM

5) Dissolution (Jacobson, 1997, 1999)
6) Reversible chemistry (various)
7) Sectional remodalization (new)



Example UAM-VPM Species

Chemical Formula	Chemical Name	Chemical Formula	Chemical Name
$H_2O(aq)$	water	Na^+	sodium ion
$H_2SO_4(aq)$	sulfuric acid	Cl^-	chloride ion
$HNO_3(aq)$	nitric acid	$Na_2SO_4(s)$	sodium sulfate
$NH_3(aq)$	ammonia	$NaHSO_4(s)$	sodium bisulfate
$HCl(aq)$	hydrochloric acid	$NaCl(s)$	sodium chloride
H^+	hydrogen ion	$NaNO_3(s)$	sodium nitrate
OH^-	hydroxy ion	$(NH_4)_2SO_4(s)$	ammonium sulfate
NH_4^+	ammonium ion	$NH_4HSO_4(s)$	ammonium bisulfate
NO_3-	nitrate ion	$NH_4Cl(s)$	ammonium chloride
HSO_4-	bisulfate	$NH_4NO_3(s)$	ammonium nitrate
SO_4^{2-}	sulfate		

Status of UAM-VPM: Plans for 2000 and beyond

- Rigorous testing of box model
- Testing of full modeling system
- Complete initial application to Vancouver for a 10-day 1993 episode
- Initiate application to Alberta

7th Conference on Air Quality Modeling: Prepared Comments on the Second Day - June 29

Joseph A. Tikvart

AMS Committee Perspective
J. Weil
AWMA Committee Perspective
R. Paine
Prognostic Meteorological Model Panel
R. Schulze
STAPPA/ALAPCO Agencies
P. Hanrahan
Department of Energy
P. Lunn
Gas Research Institute
D.Blewitt

American Petroleum Institute
H. Feldman
K. Steinberg
Utility Air Regulatory Group
A. Field
R. Paine
Southern Company
S. Vasa
Trinity Consultants
R. Schulze
Personal Statement
M. Sharan

7th Conference on Air Quality Modeling

Questions EPA Asked on New Modeling Systems

Q1. Scientific Merit

Q2. Model Accuracy

Q3. Appropriate Regulatory Applications

7th Conference on Air Quality Modeling

Questions EPA Asked on New Modeling Systems

Q4. Implementation Issues

Q5. Resource Constraints

Q6. Additional Analyses

Notes on Summary of Comments

- **Public comment period is open until 8/21/00**
- **Summary is for oral comments only**

Notes on Summary of Comments

- No responses have been formulated at this time
- Comments on the scientific merit of AERMOD, CALPUFF, and ISC-PRIME were generally favorable

Notes on Summary of Comments

- Summary of comments is based on the previous 6 questions
  - AERMOD
  - CALPUFF
  - Numerical Grid Models
  - Data from Meteorological Models
  - General Comments

Notes on Summary of Comments

- There were no specific oral comments on other models

AERMOD

Q1, Q2. Scientific Merit & Model Accuracy

- Improvements over ISC, especially regarding PBL dispersion and complex terrain, are desirable

AERMOD

Q3. Appropriate Regulatory Applications

- Add PRIME and deposition algorithms to AERMOD
- Develop AERSCREEN

AERMOD

Q4, Q6. Implementation Issues & Additional Analyses

- Define separate uses of AERMOD and ISC-PRIME
- Expand period for transition to AERMOD (>12 months)

AERMOD

Q5. Resource Constraints

- Application of PRIME -- separate from AERMOD or included with AERMOD
- Use of electronic terrain data -- need more training
- Additional EPA support

CALPUFF

Q1. Scientific Merit

- Significant advancement as State-of-Practice for long range transport
- Model flexibility provides room for growth

CALPUFF

Q2. Model Accuracy

- Testing is adequate for inclusion in the Guideline
- More testing for short-range applications is desirable

CALPUFF

Q3. Appropriate Regulatory Applications

- Appropriate for long range transport (50 - 200km)
- Need more specific guideline language for other applications

Q4. Implementation Issues

- Clarify user's guide and default options

CALPUFF

Q5. Resource Constraints

- Computer requirements
- User skills
- Additional EPA support

CALPUFF

Q6. Additional Analyses

- Requirement for 5 years of meteorological data
- Dispersion coefficient treatment
- Example protocol
- Better chemistry for SO_x/NO_x
- Overall experience of dispersion model community

Numerical Grid Models for Urban/Regional Scales

Q1. Scientific Merit

- Support removal of old grid model from guideline

Q6. Additional Analyses

- Need more testing of Models-3/CMAQ
- Insure that models are in the public domain

Data from Meteorological Models

Q1, Q2. Scientific Merit & Model Accuracy

- Use of data from meteorological models (e.g., RUC, MM5) is desirable and meets needs

Data from Meteorological Models

Q3. Appropriate Regulatory Applications

- Applications need a resolution finer than 80 km

Data from Meteorological Models

Q4. Implementation Issues

- Need detailed resolution of terrain and meteorological data
- CALMET can be used in conjunction with MM5 data
- What are the consequences of using these data bases in regulatory programs

Data from Meteorological Models

Q5. Resource Issues

- Need more modelers using RUC & MM5 meteorological model products and greater exposure to data bases

Data from Meteorological Models

- Need a repository of routine and easily accessible prognostic meteorological data (NCEP,RUC)
- Need training for MM5 and similar meteorological models

General Comments

Summary

- Public comment period is open until 8/21/00
- No responses have been formulated at this time
- Comments on the scientific merit of AERMOD, CALPUFF, and ISC-PRIME were generally favorable -- implementation / resource issues

Summary

- There were no specific comments on other models
- Next steps