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Comparison of PM2.5 Modeling Capabilities of REMSAD, MODELS-3/CMAQ, URM and CAMx

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	REMSAD	MODELS-3/CMAQ	MAQSIP	URM	CAMx	UAM-VPM
Typical Time Period	Run full year for annual average	Aggregate episodic results for annual average	Episodic, Seasonal, or Aggregate episodic results for annual average	Aggregate episodic results for annual average	Aggregate episodic results for annual average. Annual run using reduced form modules (RFM)	Aggregate episodic results for annual average
Geographic Extent	Regional (UAM-V) and urban, Continental test case: 90x56x9	Nested regional through urban, coarse grid (36-km) test case: 69x75x21	Urban to Regional. Urban test case: 45x36x15 (8-km); Regional: 69x75x21 (36-km) and 51x61x15 (28-km)	Regional and urban, SAMI Case Similar to OTAG Domain, 12-192 km multiscale mesh	Urban to continental. Variable mesh factor horizontal and vertical grid nesting	Regional and urban, Urban test case: 40x40x8 with a 40x40x8 nested grid
Computer Resources	100CPU hrs/yr (DEC Alpha, 533Mhz, 60Mb/day or 20Gb/yr)	12 CPU hrs/day (Sun Ultra30, 250Mhz, 1.4Gb/day (36-km grid)	8CPU hrs/day for the 69x75x21 case (Sun HPC 450, 250mHz), 800 Mb/day, 75 species	12CPU hrs/day (Sun Ultra2, 300Mhz, 1Gb/day: 68 gas, 13 aerosol and 8 sensitivity species)	Depends upon application and configuration. Runs on PCS and workstations (DEC, HP, IBM, SGI, SUN)	in testing, but adjustable by user choices for resolution
Gas-phase Chemistry	May-Sep: Condensed CB-IV (22 species, 10 PM species reported); Oct-Apr: lookup table to ozone obs.	RADM2 and CB-IV (SAPRC98 planned) (45 gas-phase species, 22 aerosol species)	RADM2 (59 gas-phase species, 14 aerosol species)	SAPRC93/7 (68 gas-phase species, 13 aerosol species)	CB-IV with updated isoprene and monoterpenes (40 gas-phase, 10 Aerosol species/section). SAPRC97 (80 gas-phase, 10 Aerosol species/section)	CB-IV with Isoprene Update for gas phase with extensions (37 + species), user input for aerosol mechanism and species (aqueous, solid, organic phases, e.g., 24+ aerosol species)
Aerosol Thermodynamics	Empirical algorithm	as in Regional Particulate Model (modified MARS)	MARS (modified	ISORROPIA	ISORROPIA SCAPE2 LCAERO (RFM)	EQUISOLVE (re-coded)
PM fine/PM coarse	Primary from EI; dry dep (separate settling velocities for fine and coarse, nominal size based on the same empirical size distribution used to derive the visibility parameters)	Primary from EI, size dependent dry deposition. Secondary PM-fine from gas phase reactions.	Primary from EI, size dependent dry deposition. Secondary PM-fine from gas-to-particle conversion	Primary from EI, size dependent dry deposition. Secondary PM-fine from gas phase reactions.	Primary from EI, secondary from gas-phase reactions. Size dependent deposition	Primary from EI, size dependent dry deposition, coagulation, nucleation, dissolution & condensation. Secondary PM from gas phase reactions and physical transformations. User selectable size resolution (e.g., 3 lognormal modes with 20 size fractions)

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Inorganic PM	Sulfate, nitrate, ammonium, other PM material	Sulfate, nitrate, ammonium, other PM material	Sulfate, nitrate, and ammonium	Sulfate, nitrate, ammonium, chloride, other ionics, other PM material	Sulfate, nitrate, ammonium, chloride, other ionics, other PM material	Sulfate, nitrate, ammonium, other PM material
Secondary Inorganic Aerosol Formation	gas-phase, parameterized droplet chemistry	gas-phase, droplet chemistry	gas-phase, droplet chemistry	gas-phase, droplet chemistry	gas-phase chemistry, bulk phase or size-resolved aqueous chemistry	gas-phase, aqueous reversible chemistry
Organic PM	Primary from EI	Primary from EI ; secondary from gas phase reactions	Primary from EI	Primary from EI, secondary from gas phase reactions of organic precursors using organic aerosol production fractions	Primary from EI, secondary from gas phase reactions of organic precursors using organic aerosol precursors yields	Primary from EI
Secondary Organic Formation	VOC emission fraction from EI	Lumped aerosol yields of Pandis et al., 1992 for six gas-phase precursors.	Lumped aerosol yields (Pandis et al., 1992) for six gas-phase SOA precursors	Lumped aerosol yields of Pandis et al., 1992 , extended for monoterpenes and organic lumping used in SAPRC93/7.	Semi-volatile secondary organic aerosol module of Strader et al., 1998	Lumped aerosol yields based on Pandis et. al., 1992; Aromatic yields from Odum et. Al, 1997.
Size Distribution	One PM-2.5 Fm mode; primary coarse mode (2.5 to 10)	Lognormal distribution with two modes up to 2.5 Fm and coarse mode up to PM-10 (total number of particles in each mode and mass of each species)	Lognormal distribution with two modes up to 2.5 Fm and coarse mode up to PM-10 (predicts number concentration, and third moment of diameter in each mode), mass concentrations of component species	Discrete size bins with user choice of number and size. For SAMI using 3 sizes below 2.5 Fm and 1 coarse mode for 2.5 Fm to 10 Fm (mass of each species followed)	Discrete size bins with user choice of number and size. Eight sections recommended below 2.5 Fm to 10 Fm (mass of each species followed)	User selectable number of lognormal distributions (limited by machine resources only) with stationary or full moving averages; User selectable number of discretized size bins for high resolution calculations.
Meteorology	MM4 with FDDA(IWAQM)	MM5, non-hydrostatic or hydrostatic modes, FDDA-analysis (36, 12 km), FDDA-obs. (4 km, planned)	MM5, non-hydrostatic or hydrostatic	Have used MM4, RAMS and Objective Analysis, Using RAMS for SAMI	Any modern prognostic model: MM% or RAMS with FDDA recommended	MM5, SAIMM, MC2, FDDA, user selectable resolution with nesting
Vertical Transfer/ Number of Layers	Advection, eddy diffusion, convective exchange, dry and wet dep, 9 layers (variable, w/ vertical nesting)	Vertical exchange coefficients, 21 layers, dry deposition (RADM)	Vertical exchange coefficients, variable layers (15-32 typical), dry deposition at surface	Vertical exchange coefficients, variable number of layers. Using 7 layers for SAMI, three resistance approach to dry deposition	Vertical exchange coefficients, variable number of layers. Using 12 layers for NARSTO. Wesley (1998) resistance approach to dry deposition	Advection, eddy diffusion, convective exchange, dry deposition, variable number of layers, with vertical nesting.
Cloud Dynamics and Aqueous Chemistry	Aqueous phase sulfate production coupled with gas phase H_2O_2.	Grid-resolved cloud chemistry at all scales; Sub-grid cloud chemistry and dynamics (RADM-style) at 12 and 36 km scales	Grid-resolved cloud chemistry at all scales; Parameterized sub-grid cloud chemistry and dynamics at 12 km and larger scales.	Sub-grid cloud chemistry and dynamics using RSM.	Full bulk phase or size resolved aqueous chemistry. Full 3-D distribution of cloud/liquid water content from met model	Reversible aqueous phase chemistry at all resolutions, cloud condensation nuclei

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Air Quality (I/C, B/C, Top of Domain)	Default profiles, nested, 100mbar	Default profiles (N-S-E-W), 2-3 day initialization, nested runs, all of troposphere (100 millibars)	Default profiles , 2-3 day initialization, nested runs, 100 millibars	Use interpolated fields from observations for horizontal BCs, no gradient for vertical BC, 2-3 day initialization, nested runs, for SAMI, top of domain is in lower stratosphere.	User specified 3-D initial concentrations and lateral boundary concentrations. 1-D top concentrations	User selected inputs or defaults, ramp-up days, nested runs.
Emissions	External to REMSAD, currently using enhanced EPS 2	MEPPS (SMOKE planned), BEIS2, Mobile5a, ECIP calculates plume rise	SMOKE (modified), SMOKE-BEIS2, PART5, SMOKE (EPA version, in development)	EMS-95, BEIS2, Mobile5a	Any emissions processor supporting UAM-IV format (EPS2, EMS95, SMOKE, BEIS2, GLOBEIS)	External to UAM-VPM, currently using enhanced EPS2
Point Source Treatment	plume rise	Subgrid scale treatment of plumes (PinG and plume rise)	Plume-Rise in SMOKE. Subgrid-scale treatment of plumes (PinG, SCIPUFF) under development.	Subgrid scale treatment of plumes option (PiG and plume rise)	Subgrid scale treatment of plumes option (PiG and plume rise)	Sub-grid scale treatment of plumes (P-I-G and plume rise)
Applications	Continental U.S. , evaluation underway	NE application with operational evaluation underway (one way nest 36, 12, 4); SOS/Nashville application (planned)	Eastern U.S., Western Europe, Denver Metropolitan area	SAMI application and evaluation underway (completed July, 1995 episode), Northeast, SCISSAP applications underway for PM. Gas phase applications completed for Northeast, Los Angeles.	California South Coast Air Basin and Northeastern US applications in development	Pacific Northwest application with operational evaluation underway (two-way nest 8, 4 km)
Visibility	Derived from GCV data, extinction, deciview and visual range humidity-dependent	Extinction coefficient and deciviews calculated on the fly using: Table of visual range parameters deciview: dV=10ln($/0.01), $[$km^{-1}$] Koschmieder visual range: V_r=3.91/$[km]. Deciview and visual range are size- and humidity-dependent	Extinction coefficient and deciviews calculated on the fly using Mie scattering or empirical visibility algorithms.	Done via post processing	Post Processed	External to UAM-VPM, size and species resolved data provided for simple (e.g., deciview) or complex (e.g., Mie scattering) visibility estimations.
Process analysis	None	Jeffries process analysis and integrated reaction rates analysis	Process Rate Analysis	Direct sensitivity analysis	Ozone source apportionment Direct sensitivity analysis is Jeffries process analysis in development	None in beta version, then similar to UAM-V implementation

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Photolysis Rates	Same as UAM-V treatment	Lookup table, cloud attenuation; TOMS ozone data for attenuation (when available)	Lookup Table or Tropospheric Ultraviolet and Visible Radiation Model (TUV)	Scaled to UV radiation from Met Model and/or observations	3D variation via look up table (zenith angle, altitude, ozone, column, albedo, haze, cloud cover) from NCAR TUV model. 3-D effect of clouds using RADM approach.	Same as UAM-V treatment
Advection	Smolarkiewicz or vanLeer scheme	Bott scheme or piecewise parabolic method	Horizontal Bott or Smolarkiewicz. Vertical: First-order "donor cell" scheme	Multiscale, Streamline Upwind Petrov Galerkin finite element method	Horizontal: Smolarkiewicz or Bott. Vertical: Crank Nicholson. Diffusion separated from advection.	Smolarkiewicz.
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