A NEW VERSION OF CMAQ-MADRID

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1. INTRODUCTION

Atmospheric & Environmental Research, Inc., under funding from EPRI and the California Air Resources Board, has developed the Model of Aerosol Dynamics, Reaction, Ionization and Dissolution (MADRID) and has incorporated this new aerosol module into the 2002 version of the Community Multiscale Air Quality model (CMAQ). CMAQ-MADRID[1] is now available from the Community Modeling and Analysis System (CMAS) Center with technical documentation, a user's manual and a test case[2].

The formulation of CMAQ is continuously improved by the U.S. Environmental Protection Agency (EPA) and new versions are released typically once a year. It is important to maintain consistency between CMAQ-MADRID and CMAQ and to use the most recent publicly-released version of CMAQ for CMAQ-MADRID. Accordingly, MADRID was incorporated into version 4.3 of CMAQ (September 2003 release). Benefits in terms of computational times are discussed.

A potential concern of CMAQ-MADRID is its more demanding computational requirements compared to CMAQ and other air quality models for PM. Some modifications were made to MADRID 1 to reduce the computational requirements associated with various processes without significantly altering the modeled concentrations (MADRID 1 is the most widely used version of MADRID; see Zhang et al.[1] for descriptions of MADRID 1 and MADRID 2). These modifications, combined with the use of the most recent version of CMAQ, lead to a gain in computational speed of about one order of magnitude.

2. ASSESSMENT OF COMPUTATIONAL REQUIREMENTS OF CMAQ-MADRID

We conducted some preliminary examination of computational processing times within CMAQ-MADRID 1 and CMAQ in order to identify the major reasons for the slower computational times obtained with CMAQ-MADRID 1. The version of CMAQ-MADRID 1 that is currently available from CMAS is based on the July 2002 version of CMAQ.

CMAQ-MADRID 1 and CMAQ (July 2002 version) were run for a 25-hour period (July 4, 1999) using the domain of a 1999 Southern Oxidants Study (SOS-99) simulation. The modeling domain encompasses the contiguous United States with a 32-km horizontal resolution (160 columns by 106 rows) and 19 layers for the vertical resolution. To obtain information on the improvements in computational times that can be expected from upgrading CMAQ-MADRID to the most recent version of CMAQ (version 4.3 released in September 2003), we also examined a January 2002 simulation conducted with that version of CMAQ over the central and eastern United States with a 36-km resolution (101 columns by 95 rows) and 18 layers. All simulations were conducted on AMD Athlon MP 2000+ dual-processor machines in single-processor mode.

The number of modeled and transported species is significantly greater in CMAQ-MADRID than in CMAQ because CMAQ-MADRID includes 12 biogenic secondary organic aerosol (SOA) precursors, 34 semi-volatile oxidation products and 68 biogenic SOA species. Moreover, in this application, the gas-phase RADM2 chemistry was used in CMAQ-MADRID 1 whereas CBM-IV was used in CMAQ; RADM2 has about 30 more

species than CBM-IV. A larger number of species leads to a greater computational burden.

The elapsed computational processing time after each major process was determined in terms of the user time (time actually spent in the program) and system time (time spent in the operating system on the program's behalf). Note that both of these times refer to computational processing time and not "real-time". Typically system time is much less than the user time, and the user time can approximate the total computational processing time. For the purpose of this comparison between CMAQ-MADRID 1 and different versions of CMAQ, computational processing times (central processing unit or CPU time) are reported in milliseconds (ms) per model grid cell per hour of simulation because the two CMAQ versions were applied to different domains and episodes.

The CPU times are, in increasing order, as follows:

CMAQ (September 2003 version): 2.2 ms

CMAQ (July 2002 version): 7.9 ms

CMAQ-MADRID 1 (July 2002 CMAQ version): 26.3 ms

Note that the CMAQ September 2003 version was applied with a 36-km resolution whereas the other two models were applied with a 32-km resolution. CPU times will increase slightly (by about 10%) from a 36-km to a 32-km resolution due to Courant number constraints.

The contributions of the major processes to the CPU time in each model are summarized in Table 1. Vertical diffusion (VDIFF) has the largest contribution (75%) to the large computational processing time of CMAQ-MADRID 1. More than 90% of the CPU time within the VDIFF routine is used in setting up and solving the tri-diagonal concentration matrix with the Thompson algorithm. Note that VDIFF is also the largest CPU time contributor (56%) for the July 2002 version of CMAQ. This CPU time contribution of VDIFF decreases dramatically from the July 2002 version of CMAQ to the September 2003 version. This is due to modifications made to the CMAQ vertical diffusion module in 2003 to improve computational times. CMAQ-MADRID 1 benefits from this improvement in CMAQ when we transfer MADRID to the September 2003 version 4.3 of CMAQ.

3. NEW FORMULATION FOR SECONDARY ORGANIC AEROSOL FORMATION

Secondary organic aerosols (SOA) are composed of a multitude of species, many of which are unidentified, or incompletely characterized in terms of their thermodynamic properties and their precursors. Therefore, model representation of SOA is limited by the current state of the science. The SOA module used in MADRID 1 was formulated based on empirical SOA formation data from environmental chambers; it contains 2 anthropogenic and 12 biogenic volatile precursors and 38 surrogate SOA compounds. Such a representation of SOA compounds and precursors leads to a computational burden, as shown above, that is not conducive to fast 3-D simulations over large domains and long periods. Consequently, we optimized this module to represent the salient features of SOA formation while using an abridged representation of SOA compounds and precursors to improve model speed. The strategy for optimization is based on an analysis of the modeled SOA composition to identify the relative contributions from individual precursors. Key precursors are kept while minor precursors are grouped into lumped species. The optimized formulation retains both anthropogenic precursors but represents the mixture of biogenic precursors using only 6 terpene surrogates (see Table 2). Using a 25-hour period during SOS-99 (July 4, 1999) as a case study, the benefit in terms of computational speed is approximately 40%. The abridged representation of SOA produces slightly higher SOA concentrations than the original formulation, but the difference between the two versions is negligible compared to current uncertainties in SOA precursor emissions and SOA formulations.

A detailed description of the formulation of the new SOA formation in MADRID 1 and its comparison to the original formulation is presented by Pun et al.[3]. The original SOA formulation of MADRID 1 is retained as an option in MADRID.

4. CONCLUSION

We have presented modifications to MADRID and its incorporation into the most recent publicly-available version of CMAQ (September 2003). The computational efficiency increased by about one order of magnitude without any significant alterations in modeled concentrations. Current work is ongoing to incorporate MADRID into the 2004 version of CMAQ, to introduce a plume-in-grid treatment for PM using the SCICHEM Advanced Plume Treatment (APT)[4], as well as to incorporate mercury processes[5]. An updated version of CMAQ-MADRID-APT will be available at the end of 2004.

Table 1. Comparison of CPU times for the major processes[a] in each model.

	CMAQ-MADRID (July 2002 version)	**CMAQ** (July 2002 version)	**CMAQ** (September 2003 version)
Modules			
Gas-phase chemistry	*radm2_ci4*	*cb4*	*cb4*
Solver	*mebi*	*mebi*	*Ebi*
Aqueous-phase chemistry	*RADM*	*RADM*	*RADM*
Aerosols	*MADRID1-2sec*	*ae3*	*ae3*
Advection	*ppm*	*ppm*	*Ppm*
Domain	*SE 32 km*	*SE 32 km*	*CENRAP 36 km*
NCOLS	*160*	*160*	*101*
NROWS	*106*	*106*	*95*
NLAYS	*19*	*19*	*18*
Duration (hours)	*25*	*25*	*25*
Modeling period	*4 July 1999*	*4 July 1999*	*25 January 2002*
CPU time for each process (ms/grid cell/hour)			
XADV	1.0	0.3	0.2
YADV	1.3	0.4	0.2
ZADV	0.4	0.1	0.1
HDIFF	0.2	0.1	0.0
VDIFF	19.9	4.4	0.3
CLDPROC	0.2	0.1	0.1
CHEM	1.6	1.0	0.4
AERO	0.8	1.2	0.9
OTHER	1.0	0.3	0.2
Total	26.3	7.9	2.2

(a) XADV, YADV and ZADV: advection in the X, Y and Z directions, respectively; HDIFF and VDIFF: diffusion in the horizontal and vertical directions, respectively; CLDPROC: cloud processes including chemistry; CHEM: gas-phase chemistry; AERO: aerosol processes; OTHER: other processes.

Table 2. SOA precursors and SOA species in the abridged formulation of MADRID 1 (Pun et al.[3]).

Model species	Species represented[(a)]	Oxidant(s)	Number of condensable gaseous products	Number of particulate-phase SOA species [(b)]
TOL	TOL	OH	2	2 x n
XYL	XYL	OH	2	2 x n
HUM	CRP, HUM	OH	1	n
LIM	LIM	OH	2	2 x n
APIN	APIN	OH	2	2 x n
		O_3	2	2 x n
BPIN	BPIN, CAR, SAB	OH	2	2 x n
		O_3	2	2 x n
		NO_3	1	n
TER	TER	OH	2	2 x n
OCI	OCI, LNL,TPO, TPL	OH	2	2 x n

(a) TOL: toluene; XYL: xylene; CRP: caryophyllene; HUM: humulene: LIM: limonene; APIN: α-pinene; BPIN: β-pinene; CAR: Δ-3-carene; SAB: sabinene; TER: terpinene; OC1: ocimene; LNL: linalool; TPO: terpineol; TPL: terpinolene
(b) n = number of PM size sections

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REFERENCES

1. Zhang, Y.; Pun, B.; Vijayaraghavan, K.;. Wu, S.-Y.; Seigneur, C.; Pandis, S.; Jacobson, M.; Nenes, A.;. Seinfeld, J.H. Development and application of the Model of Aerosol Dynamics, Reaction, Ionization and Dissolution, J. Geophys. Res., 2004, 109.
2. http://www.cmascenter.org/html/models.html
3. Pun, B.; Seigneur, C,; Knipping, E. Optimizing secondary organic aerosol representation in particulate matter air quality models, Regional and Global Perspectives on Haze: Causes, Consequences and Controversies, Air & Waste Management Association, Conference, 25-29 October 2004, Ashville, NC.
4. Karamchandani, P.; Seigneur, C.; Vijayaraghavan, K. Development and testing of an advanced plume-in-grid PM model, Regional and Global Perspectives on Haze: Causes, Consequences and Controversies, Air & Waste Management Association, Conference, 25-29 October 2004, Ashville, NC.
5. Seigneur, C.; Vijayaraghavan, K.; Lohman, K.; Karamchandani, P.; Scott, C. Global source attribution of mercury deposition in the United States, Environ. Sci. Technol., 2004, 38, 555-569