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MATHEMATICAL FORMULATION AND CONSIDERATION FOR CONVERTING CMAQ MODAL PARTICULATE RESULTS INTO SIZE-RESOLVED QUANTITIES

Weimin Jiang* nd Dazhong Yin
National Research Council of Canada, Ottawa, Ontario, Canada

1. INTRODUCTION

The Third Generation Air Quality Modelling System (Models-3), developed by the Environmental Protection Agency (EPA) of the United States (US), is an integrated modelling system that contains many components (EPA, 1999a). The central science model in Models-3 is the Community Multi-scale Air Quality Model, CMAQ (EPA, 1999b). Compared with other air quality models offered by the US EPA in the past, a major advantage of CMAQ is its capability in modelling the particulate matter (PM) processes in addition to gas phase processes such as ozone formation. This unique capability makes CMAQ a potential regulatory tool to address several air quality issues such as O_3, acid rain and PM at the same time, if the model can be successfully evaluated and validated.

Scientifically, the CMAQ PM component is based on the modal approach, which calculates and outputs concentrations of various chemical species in three statistical size distributions called modes. In the CMAQ output, however, there is no quantitative information on particle sizes and distributions. Therefore, the Models-3/CMAQ results are not directly comparable with size-resolved observational data, such as $PM_{2.5}$ and speciated PM concentrations measured in various size ranges. Without a scientifically defendable solution to this problem, it would not be possible to evaluate the CMAQ PM performance.

Under a project on the study of transportation-related particulate matter funded by the interdepartmental Program of Energy Research and Development in Canada, we have developed a solution to the problem. Based on the mathematical formulations that we assembled and derived, a software package, named "PMx", was developed for converting CMAQ modal particulate matter results into size-resolved quantities. The name "PMx" means that the software package can generate particulate matter quantities at any flexible size range "x" to be specified by the user. The software package contains two sub-packages for two CMAQ versions, respectively: 1. the version implemented in the Models-3 framework and released in June 1999; 2. the stand-alone version released in July 2000. For simplicity, the two CMAQ versions are referred as CMAQ_9906 and CMAQ_0007, respectively.

* *Corresponding author address*: Weimin Jiang, Room 233, M2, National Research Council Canada, 1200 Montreal Road, Ottawa, Ontario, Canada K1A 0R6; e-mail: weimin.jiang@nrc.ca

One focus of this paper is on the mathematical formulations for calculating the size-resolved quantities based on the CMAQ modal PM results. Some issues and considerations for evaluating CMAQ PM performance are also discussed on a general scientific basis so that all the discussions will be applicable to any scenarios to be modelled. We use, for illustration purposes, some results of our PM modelling in the Lower Fraser Valley (LFV) region, which includes south-west British Columbia, Canada, and north-west Washington, US. However, there is no attempt in this paper to present a specific model evaluation exercise.

2. ISSUES ON SIZE-RESOLVED PM QUANTITIES

2.1 *CMAQ PM modelling approach and output quantities*

The PM component of CMAQ is based on the modal approach, in which particle number concentrations are represented by three log-normal distributions, shown in Figure 1. Each distribution is called a mode. Therefore, there are three PM modes in CMAQ, which are named Aitken mode (i-mode), accumulation mode (j-mode), and coarse mode (c-mode), respectively (EPA, 1999b).

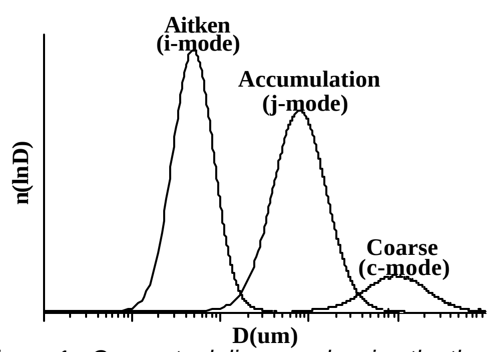

Figure 1. *Conceptual diagram showing the three PM modes modelled by CMAQ in arbitrary scale.*

CMAQ calculates and outputs mass concentrations of various chemical species and number concentrations in each mode. CMAQ_0007 also generates total surface area concentrations of the i- and j-mode particles. Table 1 lists output quantities and their units generated by the CMAQ_9906 and CMAQ_0007.

Table 1 CMAQ output PM quantities

	Models-3/CMAQ June 1999			CMAQ July 2000		
	i-mode	**j-mode**	**c-mode**	**i-mode**	**j-mode**	**c-mode**
Speciated mass concentration (mg/m^3-air)	sulphate	sulphate	marine particles	sulphate	sulphate	marine particles
	nitrate	nitrate	soil-derived particles	nitrate	nitrate	soil-derived particles
	ammonium	ammonium	other coarse particles	ammonium	ammonium	other coarse particles
	EC[a]	EC[a]		EC[a]	EC[a]	
	primary OA[b]	primary OA[b]		primary OA[b]	primary OA[b]	
	anthropogenic SOA[c]	anthropogenic SOA[c]		anthropogenic SOA[c]	anthropogenic SOA[c]	
	biogenic SOA[c]	biogenic SOA[c]		biogenic SOA[c]	biogenic SOA[c]	
	water	water		water	water	
	other primary PM2.5	other primary PM2.5		other primary PM2.5	other primary PM2.5	
Number concentration (part./m^3-air)	Yes	Yes	Yes	Yes	Yes	Yes
Surface area concentration (m^2/m^3-air)	No	No	No	Yes	Yes	No

a. EC = Elemental Carbon; b. OA = Organic Aerosols; c. SOA = Secondary Organic Aerosols

2.2 Size-resolved PM quantities needed for CMAQ evaluation

The information in Table 1 does not include size-resolved quantities, such as PM concentrations within a specified size range, which are required by most applications. Although the PM concentrations generated by CMAQ are divided into three size modes, parameters for the size distributions are not given in the CMAQ output. Without quantitative size-related information, CMAQ output is not directly comparable to size-based experimental data.

The key quantities that are needed but are missing from the current CMAQ output are the parameters of the three log-normal distributions, which include the geometric mean diameter D_g and the geometric standard deviation s_g. Based on these quantities and other properties of particles, such as density, the speciated and total concentrations in any size ranges can be calculated and compared with ambient measurement data.

3. MATHEMATICAL FORMULATION FOR CALCULATING SIZE-RESOLVED PM QUANTITIES BASED ON CMAQ PM OUTPUT

The two CMAQ versions treat size distribution parameters differently. In CMAQ_9906, D_g for each of the three PM modes changes during the atmospheric processes, while s_g for each mode is fixed. In CMAQ_0007, each D_g and s_g is variable except that the coarse mode s_g is fixed. In this section, we present mathematical formulation for calculating these quantities as well as the total and speciated concentrations in any given PM size range, using currently available CMAQ output and some internal parameters assigned in the CMAQ source code. Since the two CMAQ versions treat size distribution parameters differently, we will show the calculations in two subsections, respectively. For simplicity, only final formulas used in the calculations are presented. Details of mathematical derivations are available in the literature (Jiang and Yin, 2001).

3.1 Formulas for CMAQ_9906

Our objective is to calculate D_g, number and speciated mass concentrations in a chosen size range [*0, D**] for each mode, and the total number and mass concentrations of all particles in the size range in all modes. Particles in the size range [*0, D**] are often referred to as PMx, where x = *D**. For example, $PM_{2.5}$ refers to particles whose diameters are smaller than or equal to *D** = x = 2.5µm. (PMx or $PM_{2.5}$ sometimes also refers to the mass of the particles in the specified size range for simplicity). Prior to calculating these quantities, the third moment of each size distribution needs to be calculated, and s_g has to be extracted from the CMAQ source code.

3.1.1 The third moment $M_{3,k}$ for each mode

The third moment, M_3 ,of each mode can be calculated using the speciated PM mass concentrations in the CMAQ output and the assumed aerosol densities used in the CMAQ source code

$$M_{3,k} = \frac{6}{p} \sum_{l} \frac{Mass_{l,k}}{r_l} \qquad (1)$$

where the mode number *k* refers to i-, j-, or c-mode; $Mass_{l,k}$ is the mass concentration of the *l*-th PM species in the *k*-th mode; and r_l is the density of the *l*-th species. The species in each mode are listed in Table 1. In

CMAQ, each species is assigned a constant density, independent of the mode to which the species belongs. Table 2 shows the densities used by CMAQ. They are also used in the calculations presented in this paper.

Table 2 Densities of CMAQ PM species

PM species	Density (mg/mm^3)
sulphate	1.8 x 10^{-6}
nitrate	1.8 x 10^{-6}
ammonium	1.8 x 10^{-6}
elemental carbon	2.2 x 10^{-6}
primary organic carbon	2.0 x 10^{-6}
anthropogenic secondary organic aerosols	2.0 x 10^{-6}
biogenic secondary organic aerosols	2.0 x 10^{-6}
water	1.0 x 10^{-6}
other primary $PM_{2.5}$	2.2 x 10^{-6}
marine PM	2.2 x 10^{-6}
soil-derived PM	2.6 x 10^{-6}
other coarse PM	2.2 x 10^{-6}

3.1.2 Geometric standard deviation $s_{g,k}$ for each mode

CMAQ_9906 uses fixed $s_{g,k}$ values for each of the three modes. The values are 1.70, 2.00, and 2.20 for the i-, j-, and c-mode, respectively.

3.1.3 Geometric mean diameter $D_{g,k}$ for each mode

$D_{g,k}$ can be calculated using the formula in the literature (EPA, 1999b)

$$D_{g,k} = \left[\frac{M_{3,k}}{N_k \exp\left(\frac{9}{2} \ln^2 s_{g,k} \right)} \right]^{1/3} \qquad (2)$$

where the mode number k refers to the i-, j-, or c-mode; $M_{3,k}$ and $s_{g,k}$ are the third moment and the geometric standard deviation of the k-th mode, which are calculated and extracted as discussed before; The total particle number concentration of the k-th mode, N_k, is available in the CMAQ output.

3.1.4 Number concentration of particles in the size range [0, D] in each mode, and total number concentration of particles in the size range in all modes*

Number concentration of particles in the size range [$0, D^*$] of the k-th mode can be calculated by

$$N_k(D^*) = N_k \left\{ 1 - \frac{1}{2} erfc\left[\frac{\ln(D^*/D_{g,k})}{\sqrt{2} \ln s_{g,k}} \right] \right\} \qquad (3)$$

where k refers to the i-, j-, or c-mode; N_k is the number concentration of particles in the k-th mode, which is available in the CMAQ output; $D_{g,k}$ and $s_{g,k}$ can be calculated and extracted as explained above; *erf*c is the complementary error function (Spandier amd Oldham, 1987).

A convenient and effective way to evaluate *erfc(x)* is to use the Chebyshev approximation (Press et al., 1989)

$$\begin{aligned} erfc(x) = {} & T \exp(-Z^2 - 1.26551223 + T(1.00002368 \\ & + T(0.37409196 + T(0.09678418 \\ & + T(-0.18628806 + T(0.27886807 \\ & + T(-1.13520398 + T(1.48851587 \\ & + T(-0.82215223 + 0.17087277T))))))))) \end{aligned} \qquad (4)$$

where $Z = |x|$, and $T = 1.0 / (1.0 + 0.5Z)$.

Total number concentration of particles in the size range [$0, D^*$] in all 3 modes can be calculated by

$$N_{tot}(D^*) = \sum_k N_k(D^*) \qquad (5)$$

3.1.5 Speciated mass concentrations in the size range [0, D] in each mode, and total PMx mass concentration*

The PM mass in the size range [$0, D^*$] in a mode k, $Mass_k(D^*)$, as a fraction of the total mass in the mode k, $Mass_k$, can be calculated by

$$\begin{aligned} f_k(D^*) &= \frac{Mass_k(D^*)}{Mass_k} \\ &= 1 - \frac{1}{2} erfc\left(\frac{\ln D^* - \ln D_{g,k}}{\sqrt{2} \ln s_{g,k}} - \frac{3}{\sqrt{2}} \ln s_{g,k} \right) \end{aligned} \qquad (6)$$

where k refers to the i-, j-, or c-mode.

Assuming all particles in the same mode have the same chemical composition, then the mass concentration of particle species l in the size range [$0, D^*$] in mode k can be calculated as

$$Mass_{l,k}(D^*) = Mass_{l,k} \times f_k(D^*) \qquad (7)$$

where $Mass_{l,k}$ is the mass concentration of species l in the whole mode k, which is available in the CMAQ output.

Total mass concentration of all species in the size range [$0, D^*$] in all modes can be calculated according to the formula

$$Mass_{tot}(D^*) = \sum_k \sum_l Mass_{l,k}(D^*) \qquad (8)$$

$Mass_{tot}(D^*)$ is the total PMx mass concentration, where $x = D^*$.

3.2 Formulas for CMAQ_0007

In addition to calculating $D_{g,k}$, $N_k(D^*)$, $N_{tot}(D^*)$, $Mass_{l,k}(D^*)$ and $Mass_{tot}(D^*)$, we also need to calculate surface area concentrations of particles in the size range [$0, D^*$] for CMAQ_0007. Since the geometric standard deviations of the i- and j-modes are treated as variables in CMAQ_0007, they also need to be calculated as functions of particle number concentrations, the second moment and the third moment of the modes.

3.2.1 The third moment $M_{3,k}$ for each mode

Use Equation 1.

3.2.2 The second moment $M_{2,k}$ for each of the i- and j-modes

The second moment is closely associated with the surface area concentration of particles. $M_{2,k}$ can be calculated by the following equation

$$M_{2,k} = \frac{S_k}{p} \quad (9)$$

where S_k is the surface area concentration of the k-th mode particles, which is available in the CMAQ_0007 output.

3.2.3 Geometric standard deviation $s_{g,k}$ for each mode

The formula for calculating $s_{g,k}$ is

$$s_{g,k} = \exp\left(\sqrt{\frac{1}{3}\ln\frac{N_k M_{3,k}^2}{M_{2,k}^3}}\right) \quad (10)$$

Here k refers to the i- or j-mode. N_k is the particle number concentration in the k-th mode, which is provided by the CMAQ output. $M_{2,k}$ and $M_{3,k}$ are calculated by Equations 9 and 1, respectively.

For the coarse mode, s_g is assigned a constant value of 2.2 by CMAQ_0007. This is the same value as that used in CMAQ_9906.

3.2.4 Geometric mean diameter $D_{g,k}$ for each mode

Use Equation 2.

3.2.5 Number concentration of particles in the size range [0, D] in each mode, and total number concentration of particles in the size range in all modes*

Same formulas as in section 3.1.4.

3.2.6 Speciated mass concentration in the size range [0, D] in each mode, and total PMx mass concentration*

Same formulas as in section 3.1.5.

3.2.7 Surface area concentrations of particles in the size range [0, D] in the i- and j-modes*

Surface area concentrations of particles in the size range [0, D*] in the mode k can be expressed as

$$S_k(D^*) = S_k\left[1 - \frac{1}{2}erfc\left(\frac{\ln D^* - \ln D_{g,k}}{\sqrt{2}\ln s_{g,k}} - \sqrt{2}\ln s_{g,k}\right)\right] \quad (11)$$

where the mode number k refers to the i- or j-mode. The mode k surface area concentration, S_k, is available in the CMAQ_0007 output.

4. SIZE-RESOLVED CMAQ PM QUANTITIES CALCULATED BY THE PMx SOFTWARE

Based on the mathematical formulation presented above, we have developed two separate CMAQ post-processing sub-packages for CMAQ_9906 and CMAQ_0007, respectively, to generate size-resolved PM quantities, listed in Table 3.

5. CONSIDERATIONS FOR EVALUATING CMAQ PM PERFORMANCE

The quantities in Table 3 can be used in comparison with size-resolved ambient measurement data for CMAQ model evaluation purposes. The discussion is focused on the basis of comparing spherical particles with defined densities. For PM quantities reported in aerodynamic diameters, adjustment may be needed prior to the comparison. This subject is beyond the focus of this paper and will not be treated here.

5.1 Number concentrations

The calculated total PMx number concentration, NumConc_PMx, can be used to compare with the corresponding ambient measurement data in the chosen size range directly. However, since NumConc_PMx includes some particles from the coarse mode, which may contain mostly particles from marine and dust sources, some users may tend to use the total number of i- and j-mode particles in the PMx range if there are no significant marine and dust particles in their scenarios. The smaller the particle sizes that we consider, the smaller is the difference between the total PMx number concentration and the total number concentration of i- and j-mode particles in the PMx range, which is given by NUMATKN_PMx + NUMACC_PMx (or NumConc_PMx – NUMCOR_PMx).

5.2 Speciated mass concentration in PMx

The mass concentration of a species in PMx can be obtained by adding the species mass concentrations in all modes that contain the species. For example,

mass concentration of sulphate in $PM_{2.5}$
= ASO4I_PM2.5 + ASO4J_PM2.5

where ASO4I_PM2.5 and ASO4J_PM2.5 are calculated by specifying the upper size bound 2.5µm.

The mass concentration of a species in PMx can be compared with ambient measurement data directly.

Table 3 Sized-resolved CMAQ PM quantities [a]

	Variable name	Meaning
Geometric mean diameter (μm)	Dgi	i-mode geometric mean diameter
	Dgj	j-mode geometric mean diameter
	Dgc	c-mode geometric mean diameter
Geometric standard deviation	sgma_gi	i-mode geometric standard deviation
	sgma_gj	j-mode geometric standard deviation
	sgma_gc	c-mode geometric standard deviation
PMx mass concentration ($\mu g/m^3$-air)	MassConc_PMx	Total PMx mass concentration of all species in all modes
	ASO4I_PMx	i-mode sulphate mass concentration in PMx
	ANO3I_PMx	i-mode nitrate mass concentration in PMx
	ANH4I_PMx	i-mode ammonium mass concentration in PMx
	AECI_PMx	i-mode EC[b] mass concentration in PMx
	AORGPAI_PMx	i-mode primary OA[c] mass concentration in PMx
	AORGAI_PMx	i-mode anthropogenic SOA[d] mass concentration in PMx
	AORGBI_PMx	i-mode biogenic SOA[d] mass concentration in PMx
	AH2OI_PMx	i-mode water mass concentration in PMx
	A25I_PMx	i-mode other primary PM2.5 mass concentration in PMx
	ASO4J_PMx	j-mode sulphate mass concentration in PMx
	ANO3J_PMx	j-mode nitrate mass concentration in PMx
	ANH4J_PMx	j-mode ammonium mass concentration in PMx
	AECJ_PMx	j-mode EC[b] mass concentration in PMx
	AORGPAJ_PMx	j-mode primary OA[c] mass concentration in PMx
	AORGAJ_PMx	j-mode anthropogenic SOA[d] mass concentration in PMx
	AORGBJ_PMx	j-mode biogenic SOA[d] mass concentration in PMx
	AH2OJ_PMx	j-mode water mass concentration in PMx
	A25J_PMx	j-mode other primary PM2.5 mass concentration in PMx
	ASEAS_PMx	marine particle mass concentration in PMx
	ASOIL_PMx	soil-derived particle mass concentration in PMx
	ACORS_PMx	other coarse particle mass concentration in PMx
PMx number concentration (particle/m^3-air)	NumConc_PMx	Total PMx number concentration of particle in all modes
	NUMATKN_PMx	i-mode particle number concentration in PMx
	NUMACC_PMx	j-mode particle number concentration in PMx
	NUMCOR_PMx	c-mode particle number concentration in PMx
PMx surface area concentration[e] ($\mu m^2/m^3$-air)	SRFATKN_PMx	i-mode particle surface area concentration in PMx
	SRFACC_PMx	j-mode particle surface area concentration in PMx

a. PMx *is used in the table for generality. In a real application, a number will be used to replace* x, *e.g., PM1, PM2.5, etc.* *b. EC = Elemental Carbon; c.OA = Organic Aerosols; d. SOA = Secondary Organic Aerosols; e. PM surface areas are used only in* CMAQ_0007.

5.3 Total $PM_{2.5}$ mass concentration

The total $PM_{2.5}$ mass concentration, MassConc_PM2.5, is called "modelled PM2.5" in this paper for simplicity. The results can be compared with ambient measurement data directly. Some users may tend to use the following alternative quantities for comparison with measured $PM_{2.5}$ mass concentration data:

1. total mass concentration of all original CMAQ output species in the i- and j-modes, i.e., assuming i + j = $PM_{2.5}$. We call this approach "i+j" for simplicity.

   This has been a widely used approach among Models-3 users up to now. This approach is used for two reasons: (1) the Models-3 science manual states that $PM_{2.5}$ is treated by the i- and j-modes in CMAQ; (2) CMAQ does not provide quantitative size-related information. As we will show later, quantitative differences between the modelled PM2.5 and i+j can vary widely depending on the modelling scenario, location of the measurement, time of measurement, etc.

2. total mass concentration of all i- and j-mode species in $PM_{2.5}$, i.e., a summation of all variables starting from ASO4I_PM2.5 to A25J_PM2.5 in Table 3 (PM2.5 is used in place of PMx). We will call this approach "i_PM2.5 + j_PM2.5" for simplicity.

   This approach might be justifiable if the observed $PM_{2.5}$ mass contains negligible marine or dust–related components. However, as we will show later, the difference between the modelled PM2.5 and i_PM2.5+j_PM2.5 also varies depending on the specific modelling conditions.

Figure 2 shows conceptual differences among the modelled PM2.5, i+j, and i_PM2.5+j_PM2.5. The shaded areas in Figures 2a, 2b, 2c contain the particles whose total mass are the modelled PM2.5, i+j, and i_PM2,5+j_PM2.5, respectively.

Relative magnitude of the modelled PM2.5 and i+j depends on the relative mass of the particles in area I of Figure 2a and area II of Figure 2b. The area I is

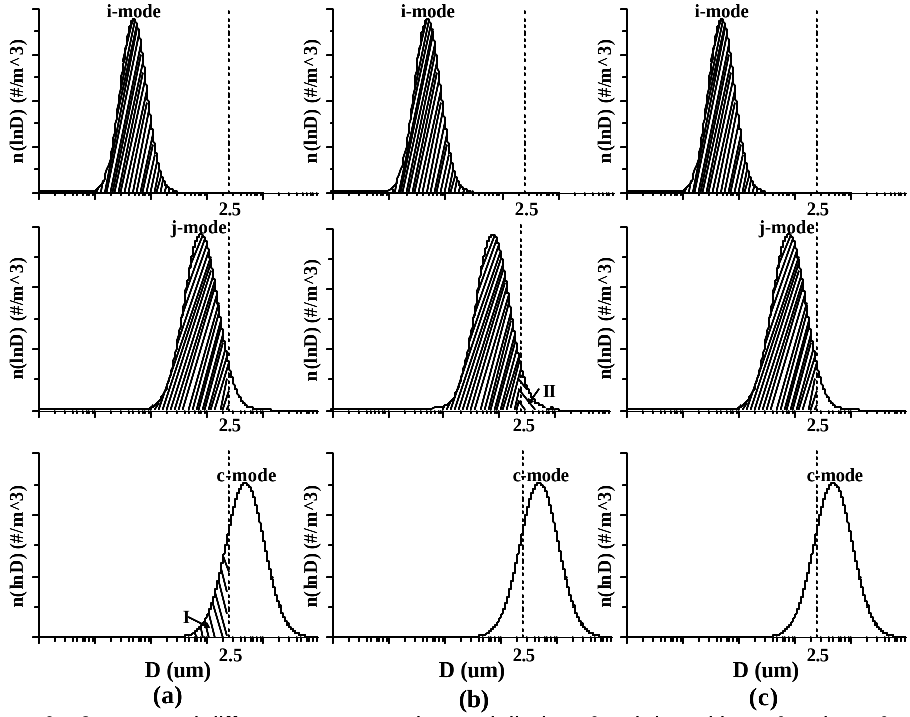

Figure 2. *Conceptual differences among the modelled PM2.5, i+j, and i_PM2.5+j_PM2.5, which are the mass of the particles covered by the total shaded areas in (a), (b), (c), respectively. Therefore, the three subfigures show: (a). the modelled PM2.5; (b) i+j; (c) i_PM2.5+j+j_PM2.5.*

covered by the c-mode and on the left of the 2.5μm line in Figure 2a, while the area II is covered by the j-mode and on the right of the 2.5μm line in Figure 2b. Mathematically, the i-mode curve also extends beyond the 2.5μm line, and there is also an area II under the i-mode curve that is similar to the one under the j-mode curve. In practice, the area II under the i-mode curve is too small to be seen so that it can be ignored. Generally, the mass of the particles in areas I and II can vary widely. Therefore, the difference between the modelled PM2.5 and i+j can also change widely based on the modelling conditions. However, if the mass of the particles in area I is approximately equal to the mass in area II, then the modelled PM2.5 will be approximately equal to i+j. Under this condition, the alternative approach 1 may give similar values to the modelled PM2.5 and i+j for an incorrect reason.

Theoretically, the modelled PM2.5 or i+j are always larger than i_PM2.5+j_PM2.5. However, when the mass of the particles in area I of Figure 1a is negligible, the modelled PM2.5 will be very close to i_PM2.5+j_PM2.5. Considering that the area I belongs to coarse mode particles that are mostly from sources different from the i- and j-mode particle sources, the alternative approach 2 may be valid under this situation.

Figure 3 gives an example of differences among the modelled PM2.5, i+j, and i_PM2.5+j_PM2.5 for a modelling scenario in the Lower Fraser Valley. The values shown in Figure 3 are the three PM quantities averaged over all cells in the modelling domain for each of the 191 modelling hours from 1:00 July 31 to 24:00 August 7, 1993.

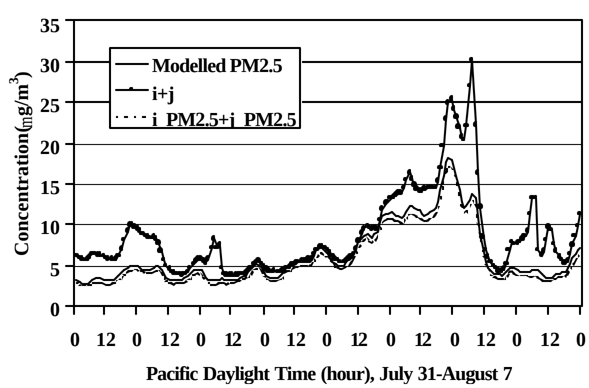

Figure 3. *An example of the differences among the modelled PM2.5, i+j, and i_PM2.5+j_PM2.5. The data were based on the output from a CMAQ_0007 run for the Lower Fraser Valley, which includes south-west British Columbia in Canada and north-west of Washington in the US, for the period of July 31 to August 7, 1993. The CMAQ output was converted into the size-resolved quantities using the PMx software, which is based on the mathematical formulation discussed in this paper.*

The LFV modelling data are used for the purpose of helping to visualise the magnitude of the differences among the quantities only, and the real geographical location of the modelling domain is irrelevant here.

Therefore the map of the domain is omitted. More information on our LFV modelling domain is available in other documents, such as Jiang et al., 2001.

In this particular example, the average modelled PM2.5 and i_PM2.5+j_PM2.5 are close to each other for all the modelling hours. This is due to the fact that the average area I in Figure 2a is very small throughout the modelling period. The coarse mode particles are mostly distributed well above the 2.5μm line. In contrast, the i+j curve in Figure 3 is generally above the curves for the modelled PM2.5 and i_PM2.5+j_PM2.5. The difference between the i+j curve and modelled PM2.5 curve also varies widely during the modelling period.

Table 4 shows the maximum, minimum, and average differences between i+j and the modelled PM2.5, and between i_PM2.5+j_PM2.5 and the modelled PM2.5 for the modelling period. Both absolute and relative differences are shown in the table. In all the calculations, the modelled PM2.5 is used as the base value. i+j can be 16.43 μg/m^3 higher than the modelled PM2.5 at one hour, and can also be slightly lower (0.05 μg/m^3 lower) at another hour. In relative terms, i+j is 211% higher than the modelled PM2.5 when the relative difference between i+j and the modelled PM2.5 is at the maximum. It is just 0.98% lower than the modelled PM2.5 when the relative difference is at the minimum. Averaging over the whole modelling period, i+j is 44.6% higher than the modelled PM2.5. In contrast, the differences between i_PM2.5+j_PM2.5 and the modelled PM2.5 are much smaller.

Table 4 Differences between average hourly values of i+j and modelled PM2.5, and between i_PM2.5+j_PM2.5 and modelled PM2.5

	i+j vs. modelled PM2.5		i_PM2.5+j_PM2.5 vs. modelled PM2.5	
	μg/m^3-air	%	μg/m^3-air	%
Maximum	16.43	211.12	-0.19	-4.55
Minimum	-0.05	-0.98	-1.07	-17.64
Average	2.45	44.6	-0.56	-10.17

The results in Table 4 only show the situations under our modelling conditions on a domain-average basis. The results may change dramatically if the PM quantities in individual grid cells are examined, or a different scenario is modelled for a different domain. The key point that we would like to make here is that the modelled PM2.5 values have to be calculated for model evaluation purpose. Without the knowledge of quantitative size distributions, we would not be able to know how close an alternative quantity, such as i+j, can be in comparison with the modelled PM2.5.

5.4 Total PMx other than $PM_{2.5}$

Using the formulas described in this paper, PM mass and number concentrations in any chosen size ranges can be calculated and compared with the corresponding ambient measurement data. The results of the comparison will show if the assumption of log-normal distribution of PM sizes, which is the basis of the modal approach, is reasonable for the modelling scenario under investigation. This information is extremely useful in getting a complete picture of the model performance across a wide spectrum of size ranges. If the results are reasonable and satisfactory, they will greatly increase the confidence level in using Models-3/CMAQ and the modal approach for the PM study.

6. SUMMARY

In this paper, we have presented the mathematical formulation for converting CMAQ modal particulate matter results into size-resolved quantities, and some considerations for PM performance evaluations. Considering the rapidly increasing interest in Models-3/CMAQ from the air quality modelling community, policy makers, and industrial users, it is extremely important to ensure that the modelling system is correctly evaluated and validated. The mathematics and discussions are widely applicable to other PM models that are based on the modal approach.

7. ACKKNOWLEDGEMENT

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APPENDIX: NOTATION

D^*	upper bound of a particle size diameter range, μm
D_g	geometric mean diameter of a particle number distribution, μm
$D_{g,k}$	geometric mean diameter of the mode *k* particle number distribution, μm
erfc	the complementary error function
$f_k(D^*)$	mass in the size range [*0, D**] in mode *k* as a fraction of all mass in mode *k*
$M_{2,k}$	the *2*nd moment of mode *k*, $\mu m^2/m^3$-air
$M_{3,k}$	the *3*rd moment of mode *k*, $\mu m^3/m^3$-air
$Mass_{l,k}$	mass concentration of species *l* in mode *k*, $\mu g/m^3$-air
$Mass_k$	mass concentration of particles in mode *k*, $\mu g/m^3$-air
$Mass(D^*)$	mass concentration of particles in the size range [*0, D**] in a mode, $\mu g/m^3$-air
$Mass_{l,,k}(D^*)$	mass concentration of species *l* in the size range [*0, D**] in mode *k*, $\mu g/m^3$-air
$Mass_k(D^*)$	mass concentration of particles in the size range [*0, D**] in mode *k*, $\mu g/m^3$-air
$Mass_{tot}(D^*)$	total mass concentration of particles in the size range [*0, D**] in all modes, $\mu g/m^3$-air
N_k	number concentration of particles in mode *k*, particle/m^3-air
$N_k(D^*)$	number concentration of particles in the size range [*0, D**] in mode *k*, particle/m^3-air
$N_{tot}(D^*)$	total number concentration of particles in the size range [*0, D**] in all modes, particle/m^3-air
S_k	surface area concentration of particles in mode *k*, $\mu m^2/m^3$-air
$S_k(D^*)$	surface area concentration of particles in the size range [*0, D**] in mode k, $\mu m^2/m^3$-air
r_l	density of species *l* in particles, $\mu g/\mu m^3$
s_g	geometric standard deviation of a mode
$s_{g,k}$	geometric standard deviation of mode *k*