APPROACH FOR MODELING POM

Issues with modeling POM

Not all POM reported to EPA's national emission inventory (NEI) are speciated into individual compounds. As a result, we must apply some simplifying assumptions in order to model and assess the risk from the individual pollutants that comprise POM. This involves establishing different POM "groups" and modeling them as separate pollutants. In establishing these groups, we considered the need to provide the most detailed information about risks from the individual pollutants within POM while taking into account the inconsistencies in how much speciation is reported in the inventory. We used a more refined method to establish POM groups for the 1999 NATA than we did for the 1996 NATA to reflect improvements in the speciation of POM within the inventory. Specifically, for the 1996 NATA we had two overlapping POM groups and for the 1999 NATA we have eight distinct groups.

1996 NATA Approach

For the 1996 NATA, we had two POM groups: (1) 7-PAH and (2) total POM. Note that the two groups overlap one another in that the total POM also contains pollutants in the 7-PAH group. We chose these groups in order to provide a range of the risk estimate. This is because the bulk of the POM was reported in the inventory as unspeciated POM. In addition, in some cases, the inventory contained more than one PAH group for the same stack (e.g., unspeciated POM, unspeciated 7-PAH in the same stack). For 7-PAH, we included only those pollutants that either were individual constituents of the 7-PAH group, such as benzo(a)pyrene, or were reported as "7-PAH" in the inventory. This would potentially be the low range since it did not include any pollutants identified as total POM, which presumably include some 7-PAH. The total POM group included all individual compounds belonging to POM as well as unspeciated POM and PAH groups. In addition, the total POM group included the compound "naphthalene" which is listed as a separate HAP in the Clean Air Act list of 188, but was not inventoried this way in the 1996 inventory. The total POM group could conceivably double count emissions from stacks in which multiple POM groups were reported. Additional explanations for the approach can be found in Appendix D of the EMS-HAP User's Guide, Version 2.0, which can be downloaded from www.epa.gov/ttn/emch/models. An explanation of the risk assumptions for these two groups can be found at http://www.epa.gov/ttn/atw/nata/nettables.pdf. As is stated in the latter document, the risk from the 7-PAH group was found to be significantly lower than that from the total POM group, and the 7-PAH group was subsequently dropped from the assessment.

1999 NATA Approach

For the 1999 NATA, we used a very different, more refined approach to group POM to reflect the improvements in the inventory. There are three main 1999 NEI improvements related to POM. First, a larger quantity of the 1999 NEI emissions is speciated into individual POM compounds. Second, there is no double-counting of POM groups from individual stacks in the point source inventory. There was still an inventory issue relating to double counting of 7-PAH and 16-PAH from numerous non-point sources (e.g., animal cremation, human cremation) and nonroad (e.g., 2-stroke logging equipment). We fixed this issue prior to ASPEN modeling by creating a "new" inventory pollutant, whose emissions are the difference between 16-PAH and 7-PAH. Third, naphthalene is inventoried as a separate HAP and is not included nor summarized in any PAH group.

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The approach taken to assess POM for the 1999 NATA is to group inventory POM species into non-overlapping categories for which we can associate similar inhalation risks based on the unit risk estimate (URE). Unit risk estimates were obtained from the toxicity table http://www.epa.gov/ttn/atw/toxsource/table1.pdf (version dated October 2003) for the individual POM compounds. Table 1 shows the 8 POM groups and the associated URE assignments. Note that naphthalene is not included within any of the 8 POM groups for the 1999 NATA. For the 1999 NATA, naphthalene is modeled and treated as a separate HAP; it is not combined with other pollutants considered to be POM.

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Table 1. POM groups for the 1999 National Scale Air Toxics Assessment

POM GROUP (EMS-HAP code)	Names Used in NATA Website	Description of Group	URE for Risk Charact-erization	Basis for URE
71002	POM, Group 1: Unspeciated POM_Group_1_unspec	Group contains unspeciated POM, no URE is associated with them	$5.5 * 10^{-5}$	Assume same URE as was assumed for total POM group in NATA 1996: 5% of risk from Benzo(a)pyrene
72002	POM, Group 2: No URE data POM_Group_2_nodata	Group contains individual POM species that have no URE associated with them	$5.5 * 10^{-5}$	Assume same URE as is used for unspeciated POM (71002)
73002	POM, Group 3: 5e-2<URE<5e-1 POM_Group_3_vhigh1	Group contains individual POM species in which the UREs are between: 5e-2<URE<5e-1	$1 * 10^{-1}$	Midpoint of range
74002	POM, Group 4: 5e-3<URE<5e-2 POM_Group_4_high2	Group contains individual POM species in which the UREs are between: 5e-3<URE<5e-2	$1 * 10^{-2}$	Midpoint of range
75002	POM, Group 5: 5e-4<URE<5e-3 POM_Group_5_mhigh3	Group contains individual POM species in which the UREs are between: 5e-4<URE<5e-3	$1 * 10^{-3}$	Midpoint of range; note this is the group that contains Benzo(a)pyrene
76002	POM, Group 6: 5e-5<URE<5e-4 POM_Group_6_med4	Group contains individual POM species in which the UREs are between: 5e-5<URE<5e-4	$1 * 10^{-4}$	Midpoint of range
77002	POM, Group 7: 5e-6<URE<5e-5 POM_Group_7_mlow5	Group contains individual POM species in which the UREs are between: 5e-6<URE<5e-5	$1 * 10^{-5}$	Midpoint of range
78002	POM, Group 8: Unspeciated 7-PAH POM_Group_8_Unspec_7	Group contains pollutant reported as "7-PAH"	$2 * 10^{-4}$	Assume same URE as was used for 7-PAH from 1996 NATA, 18% of of risk from Benzo(a)pyrene

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Table 2 shows the assignment of the POM in the 1999 NEI to the eight POM modeled pollutant groups. Note that summaries of POM in the 1999 NEI are provided for a different set of groups that don't have a one-to-one relationship to the modeled groups. Column 4 of Table 2 shows how the 1999 NEI POM groups relate to the modeled groups. Table 2 also shows the nationwide (50 States, Puerto Rico and Hawaii) emissions of the various POM reported in the inventory[1]. In Table 2, the pollutant called "16-PAH-7-PAH" was created from the 1999 NEI version 3 prior to modeling by subtracting 7-PAH (inventory pollutant code 40) from 16-PAH (inventory pollutant code 75). It was assigned a pollutant code of 75040, but because it is not in the NEI, it does not have an associated "POM category in 1999 NEI" entry.

Table 2. Mapping of NEI HAPs belonging to POM into the modeled POM groups And 1999 NEI National-level Emissions

POM group	Pollutant code	Description of Pollutant	POM category in 1999 NEI	Point inventory	Non-point inventory	Onroad inventory	Non-road inventory	Total
				Tons/Year				
71002	103	Benz(a)Anthracene/Chrysene	POM as 7-PAH	0	0.00267	0	0	0.00267
71002	234	total PAH	POM as 7-PAH	54.85	976.96	0	0	1031.81
71002	246	Polycyclic Organic Matter	POM as 7-PAH	3314.58	644.09	0	0	3958.67
71002	40	16-PAH	POM as non-15 PAH	13.12	320.38	0	0	333.5
71002	75040	16PAH-7PAH		0	132.42	0	1.4012	133.8212
72002	120127	Anthracene	POM as 15-PAH	38.1	332.92	31.91	15.2	418.13
72002	129000	Pyrene	POM as 15-PAH	399.16	617.33	46.37	35.2	1098.06
72002	191242	Benzo[g,h,i,]perylene	POM as 15-PAH	2.04	283.7	9.35	9.91	305
72002	192972	Benzo[e]pyrene	POM as non-15 PAH	0.59	184.69	0	0	185.28
72002	195197	Benzo(c)phenanthrene	POM as non-15 PAH	0	152.71	0	0	152.71
72002	198550	Perylene	POM as non-15 PAH	2.3	35.4	0	0	37.7

1 Also note that the non-point inventory benzo-a-pyrene emissions in Table 2, which are based on the 1999 NEI version 3.0 (Fall 2003) are greatly overestimated. After the initial ASPEN modeling was completed, it was found that the State of Oregon mistakenly used a wrong emission factor for estimating its wildfire emissions (SCC = 2810001000) that caused an overestimation of benzo(a)pyrene by about factor of 4. The ASPEN results were adjusted to reflect this error, but the emissions were not changed.

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POM group	Pollutant code	Description of Pollutant	POM category in 1999 NEI	Point invent-tory	Non-point invent-ory	Onroad invent-ory	Non-road invent-ory	Total
				Tons/Year				
72002	203123	Benzo(g,h,i)Fluoranthene	POM as non-15 PAH	0	7.5	0	0	7.5
72002	203338	Benzo(a)fluoranthene	POM as non-15 PAH	0.000017	101.81	0	0	101.81
72002	206440	Fluoranthene	POM as 15-PAH	231.63	523.85	33.26	30.49	819.23
72002	208968	Acenaphthylene	POM as 15-PAH	1.42	1744.67	139.2	66.04	1951.33
72002	2381217	1-Methylpyrene	POM as non-15 PAH	0	354.36	0	0	354.36
72002	2422794	12-Methylbenz(a)Anthracene	POM as non-15 PAH	0	0.51	0	0	0.51
72002	247	Methylbenzopyrenes	POM as non-15 PAH	0.000035	114.51	0	0	114.51
72002	248	Methylchrysene	POM as non-15 PAH	0	305.61	0	0	305.61
72002	26914181	Methylanthracene	POM as non-15 PAH	0.63	322.43	0	0	323.06
72002	56832736	Benzofluoranthenes	POM as 7-PAH	0.03	205.14	0	0	205.17
72002	779022	9-Methylbenz(a)Anthracene	POM as non-15 PAH	0	1.01	0	0	1.01
72002	832699	1-Methylphenanthrene	POM as non-15 PAH	0	7.58	0	0	7.58
72002	83329	Acenaphthene	POM as 15-PAH	39.77	309.59	26.42	26.07	401.85
72002	85018	Phenanthrene	POM as 15-PAH	175.02	1085.44	90.99	100.74	1452.19
72002	86737	Fluorene	POM as 15-PAH	59.73	254.13	55.29	51.32	420.47
72002	91576	2-Methylnaphthalene	POM as non-15 PAH	9.53	20.76	0	0	30.29
72002	91587	2-Chloronaphthalene	POM as non-15 PAH	0.09	0.000000737	0	0	0.090001
73002	57976	7,12-Dimethylbenz[a]anthracene	POM as non-15	0.1	1.93	0	0	2.03

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POM group	Pollutant code	Description of Pollutant	POM category in 1999 NEI	Point invent-tory	Non-point invent-ory	Onroad invent-ory	Non-road invent-ory	Total
				Tons/Year				
			PAH					
74002	189559	Dibenzo[a,i]pyrene	POM as non-15 PAH	0.00000176	0	0	0	1.76E-06
74002	189640	Dibenzo[a,h]pyrene	POM as non-15 PAH	0.0000169	0	0	0	1.69E-05
74002	56495	3-Methylcholanthrene	POM as non-15 PAH	0.00016	0.25	0	0	0.25016
75002	192654	Dibenzo[a,e]Pyrene	POM as non-15 PAH	0.000954	0	0	0	0.000954
75002	3697243	5-Methylchrysene	POM as non-15 PAH	0.00021	0.00000405	0	0	0.000214
75002	50328	Benzo[a]pyrene(7PAH)	POM as 7-PAH	15.67	1073.9	4.84	3.19	1097.6
75002	53703	Dibenzo[a,h]anthracene	POM as 7-PAH	0.87	7.12	0.000985	0.07	8.060985
76002	102	Benzo[b+k]fluoranthene	POM as 7-PAH	0.01	0.19	0	0	0.2
76002	193395	Indeno[1,2,3-c,d]pyrene	POM as 7-PAH	0.43	178.2	2.58	3	184.21
76002	205823	B[j]fluoranthen	POM as non-15 PAH	0.001363	0	0	0	0.001363
76002	205992	Benzo[b]fluoranthene	POM as 7-PAH	4.95	85.87	5.32	2.57	98.71
76002	207089	Benzo[k]fluoranthene	POM as 7-PAH	2.07	143.53	5.32	2.37	153.29
76002	224420	Dibenzo[a,j]Acridine	POM as non-15 PAH	0.0001	0	0	0	0.0001
76002	56553	Benz[a]anthracene	POM as 7-PAH	109.4	433.97	7.97	4.85	556.19
77002	218019	Chrysene	POM as 7-PAH	30.23	388.2	4.18	3.09	425.7
78002	75	7-PAH	POM as 7-PAH	66.26	39.96	0	1.38069	107.6007