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Modelling of aerosol processes in plumes

By MIHALIS LAZARIDIS[1]*, SASTRY S. ISUKAPALLI[2] and PANOS G. GEORGOPOULOS[2],
[1]*Norwegian Institute for Air Research (NILU) Postboks 100, N-2027, Kjeller, Norway;* [2]*Environmental and Occupational Health Sciences Institute, 170 Frelinghuysen Road, Piscataway, NJ 08855, USA*

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ABSTRACT

A modelling platform for studying photochemical gaseous and aerosol phase processes from localized (e.g., point) sources has been presented. The current approach employs a reactive plume model which extends the regulatory model RPM-IV by incorporating aerosol processes and heterogeneous chemistry. The physics and chemistry of elemental carbon, organic carbon, sulfate, nitrate, ammonium material of aerosols are treated and attributed to the PM size distribution. A modified version of the carbon bond IV chemical mechanism is included to model the formation of organic aerosol. Aerosol dynamics modeled include mechanisms of nucleation, condensation, dry deposition and gas/particle partitioning of organic matter. The model is first applied to a number of case studies involving emissions from point sources and sulfate particle formation in plumes. Model calculations show that homogeneous nucleation is an efficient process for new particle formation in plumes, in agreement with previous field studies and theoretical predictions. In addition, the model is compared with field data from power plant plumes with satisfactory predictions against gaseous species and total sulphate mass measurements. Finally, the plume model is applied to study secondary organic matter formation due to various emission categories such as vehicles and the oil production sector.

1. Introduction

The evaluation and assess of the physico-chemical processes responsible for the spatial and temporal variability of photochemical pollutants and fine particles in local plumes and their effect on their long-range transport characteristics is an important scientific area and has been a very active area in the 70's and 80's (Hegg and Hobbs, 1980; Hegg et al., 1985; Whitby, 1978; Van Valin and Pueschrl, 1981, Seigneur et al., 1997, Zannetti, 1990). Plume research has not received similar attention as the development of larger-scale dispersion models during the recent years. Until recently plume models were focusing mainly on the modelling of gaseous species in the atmosphere. However, concentrations of fine particulate matter (PM) in the atmosphere are being recognized more and more as a major health concern, thus necessitating the detailed study of processes leading to the formation of PM. Relatively few modeling studies have examined the combined dynamics of gaseous and particulate matter processes in reactive plumes (Wexler et al., 1994; Hudischewskyj and Seigneur, 1989, Seigneur et al., 1997).

The main objective of the current work is the development of a mechanistic plume model that incorporates physical and chemical photochemical gaseous and particulate matter (PM) processes that can be applied to evaluate the effect of industrial stack emissions on local PM concentrations, and the associated environmental consequences. The current reactive plume model with aerosol chemistry is developed as an extension to

* Corresponding author.
e-mail: mihalis.lazaridis@nilu.no

an existing regulatory plume model, the reactive plume model, version IV (Research Triangle Park, 1992). Modifications to the original model include the addition of modules that describe aerosol chemistry, nucleation and condensation processes, while retaining the basic structure of RPM-IV (Lazaridis et al., 1998). The model considers a control volume that moves and expands downwind along the plume trajectory, and solves the dispersion/reaction equations that incorporate mechanisms for nonlinear photochemistry. It describes short term behavior of the plume, typically ranging from 1 hour to less than 24 h. Further details explaining the formulation of RPM and other reactive plume models can be found in the literature (Seinfeld, 1986; Liu et al., 1982; Georgopoulos and Seinfeld, 1989; Zannetti, 1990).

In the present paper, simulations first were performed for investigating the potential of new particle formation from a single plume for several SO_2 plume concentrations. The model is applied to study aerosol behavior following particulate matter (PM) and gaseous emissions from a single point source plume and to assess the potential of new sulfate particle formation inside plumes (Lazaridis et al., 1998). The modeling studies predicted high nucleation rates of sulfate particles close to plume sources, in agreement with the data from field studies (Hegg and Hobbs, 1980; Hegg et al., 1985; Whitby, 1978; Van Valin and Pueschrl, 1981) and with modeling analyses (Kerminen and Wexler, 1996). Furthermore, the model is applied here against several field studies from the Mohave and Navajo power plants. Comparison of the plume model with available field data is satisfactory.

Finally, the model is used to estimate production of secondary organic matter (condensible organic compounds, COC) during emissions from different emission categories in order to determine the potential of COC formation from various sources (vehicle emissions and the oil production sector). These studies were performed to investigate their potential on the formation of secondary organic matter.

In the following sections, we present shortly the main characteristics of the plume model as well as comparison with several field studies from power plant plumes in the USA. Simulations including typical emission scenarios from urban traffic and the oil sector were performed for investigating their COC potential since an important part of the aerosol particles in the atmosphere is composed by secondary formed organic matter (Turpin and Huntzicker, 1991; Lazaridis, 1999).

2. Reactive plume model with aerosols: model description

The aerosol plume model described in the current paper is an extension of the regulatory model reactive plume model (RPM), developed to simulate the atmospheric processes and dynamics of particulate matter following emissions from point source plumes. The model adopts a trajectory-based framework, where the plume emissions are divided into cells containing equal masses, according to a Gaussian plume evolution (Seinfeld, 1986). The cells travel downwind, and expand in a way such that the amount of a (fictitious) emitted inert species remains constant within each cell.

The width and the depth of the cells are computed as functions of horizontal and vertical dispersion parameters. The chemistry term is solved using the carbon-bond mechanism, version IV (Whitten et al., 1980) (CB-IV) as a default; however the user can input any alternative description of atmospheric photochemistry. The carbon-bond mechanism is a set of generalized reactions and rate constants for modeling photochemical oxidant formation. This mechanism lumps together similarly bonded carbon atoms, resulting in a condensed mechanism that is used widely in regulatory photochemical models.

2.1. *Modeling of the aerosol processes*

The plume model can quantify the relationships between point source emissions and primary and secondary aerosol species formation and dynamics under various meteorological conditions. Emissions of gaseous species (NO_x, SO_2, NH_3, VOC, CO) and primary PM (elemental carbon (EC), organic carbon (OC), crustal material, and H_2O) are inputs to the model. Gaseous phase chemistry is treated using a modified version of the carbon bond IV (CB-IV) chemical mechanism (Lurmann et al., 1997) that considers the gas/particulate matter partitioning of organic material. The chemistry of inorganic aerosols is not yet incorporated in the model. The inorganic multicomponent

atmospheric equilibrium model (SEQUILIB) (Pilinis and Seinfeld, 1987; Lurmann et al., 1997) for calculation of the aerosol component of ammonium, chloride, nitrate, sulfate and water species is considered to be included.

The aerosol size distribution and chemical composition is modeled using 16 aerosol-size bins for the PM_{10} aerosol, where the size distribution employs a nodal point scheme (Lazaridis and Koutrakis, 1997). In addition to the equilibrium scheme used above (i. e. CB-IV chemical mechanism) an aerosol dynamics approach is also developed. Processes such as nucleation, condensation and deposition are incorporated in the aerosol dynamics modules of the plume model. In the simulations performed in the present paper for studying the formation of sulfate particles near point sources of SO_2, mechanistic models for nucleation and condensation of the binary sulfuric acid–water system were included. In addition, aqueous phase oxidation of SO_2 is included in the model using a semiempirical fog model which is adopted from the UAM-AERO model (Lurmann et al., 1997) (see also Lazaridis and Skouloudis (1999)). The gaseous phase sulfate chemistry has been included in the modified CB-IV chemical mechanism.

Gas-particle partitioning of organic compounds in the atmosphere is an important step in determining their association with fine particulate matter. The current plume model adopts a method which is similar to the one employed in the UAM-AERO model (Lurmann et al., 1997), where the condensible organic compound (COC) yields for the lumped organic compounds are obtained from Pandis et al. (1992). A flexible gas-phase chemical mechanism interface that allows user modification is adopted, with the Carbon Bond IV (CB-IV) chemical mechanism (Gery et al., 1988) as the default option.

The model used for the COC formation assumes constant yield. This method gives a first-order estimate for the formation of particulate organics and is a widely used, well documented methodology and easy to be implemented in chemistry modules of existing air quality models. However, both theory and smog chamber experiments (Pankow, 1994; Odum et al., 1996; Bowman et al., 1997) show that the COC formation is not constant and varies based on the concentration of suspended matter, on atmospheric conditions and can be described with the help of the adsorption/absorption processes. The reason for following the yield approach in the current paper is for simplicity reasons due to the great complexity of the number of different chemical forms of organic matter and because it is accurate and in first order agreement with smog chamber experiments and in addition easy to be implemented in existing chemical mechanisms such as the CB-IV chemical mechanism.

Modelling of the aerosol size distribution proceeds in a manner similar to that adopted by Lazaridis and Koutrakis (1997). In the calculations focused on the new particle formation from SO_2 emissions in plumes we use a typical aerosol distribution of continental air (Lazaridis and Koutrakis, 1997; Hering and Friendlander, 1982) for describing the background size distribution. We have used a size distribution of 16 aerosol-size bins for the PM_{10} aerosol range. In the description of the background size distribution we employed a nodal point scheme Lazaridis and Koutrakis (1997): in this method the number distribution is divided into $n-1$ nodal points distributed evenly according to the logarithm of particle radius r_i. The average chemical composition for particles in nodal point i is used, i.e., all particles at a nodal point i are assumed to have the same chemical composition. The allocation of the condensible mass on the aerosol size distribution in each time step is performed using the concept of condensible fraction for each size bin.

2.2. *Aerosol dynamics*

The plume model has the capability to calculate the binary nucleation process for the H_2SO_4–H_2O system. The nucleation process of additional gaseous species can be easily implemented provided that the necessary thermodynamic properties are available. The binary nucleation of the H_2SO_4–H_2O system is calculated in a manner analogous to the one provided by the revised classical theory (Lazaridis and Drossinos, 1997).

The condensation rate of H_2SO_4 onto the preexisting aerosol particles is described by a modified Mason equation, which includes the transitional correction factors (Lazaridis and Koutrakis, 1997). There are recent theoretical and observational evidence that the presence of ammonia in the atmosphere can accelerate greatly the binary

nucleation rate of sulfuric acid - water (Weber et al., 1999; Ball et al., 1999; Korhonen et al., 1999). This will have implications on the new particle formation rate inside plumes in situations that the ambient ammonia levels are in the range of several ppt (Korhonen et al., 1999). Therefore, the present predictions on the new particle formation capacity inside plumes can considerably underestimate the actual particle formation in areas with elevetated ammonia concentrations.

In the plume model, two alternative methods are used to describe the mechanism of dry deposition for particles and gaseous species. The first method utilizes available experimental data for different species (Seinfeld, 1986). The second method is based on quantifying the transfer of material from the atmosphere to the surface through different resistance mechanisms, i.e., the aerodynamic resistance, the surface resistance, and the transfer resistance (Slinn and Slinn, 1980). A similar method is used by the UAM-AERO model (Lurmann et al., 1997). The model provides the user with the option to include a mechanism of wet deposition and consider the effect of wet scavenging of particles in a part of the whole modeling domain. The rate of scavenging can be estimated via use of the washout coefficient (Finlayson-Pitts and Pitts, 1986).

The dry deposition velocity of aerosol particles in the present work is calculated with the resistance method using the following equation (Slinn and Slinn, 1980):

$$v_{\mathrm{d}}^{i} = \frac{1}{r_{\mathrm{a}} + r_{\mathrm{d}}^{i} + r_{\mathrm{a}} r_{\mathrm{d}}^{i} v_{\mathrm{g}}} + v_{\mathrm{g}}^{i}, \qquad (1)$$

where v_{d}^{i} is the deposition velocity (m/s) of particles of the ith size bin, r_{a} is the aerodynamic resistance (s/m), r_{d}^{i} is the deposition layer resistance (s/m) of particles of the ith size bin and v_{g}^{i} is the gravitational settling velocity (m/s) of particles of the ith size bin.

Primary emissions of particulate matter (PM) from point sources have to be supplied as inputs, including information for size distribution/chemical composition.

3. Results and discussion

The plume model is applied first here to study new sulfate particle formation in plumes due to homogeneous nucleation of the sulfuric acid–water system. Furthermore, several comparisons between model predictions and field studies were performed for investigating the capability of the current plume model to simulate gaseous and aerosol concentration characteristics close to point sources. Finally, the model is used to study secondary organic matter formation during emissions from vehicles and also from the offshore oil industry activities.

3.1. New particle formation in plumes

In a number of field studies a high production of new particles was observed (Hegg and Hobbs, 1980; Hegg et al., 1985; Whitby, 1978; Vanvalin and Pueschrl, 1981). Kerminen and Wexler (1996) used a Gaussian plume model to study the nucleation probability in plumes and new particle formation was predicted in a number of spatial patterns for different initial conditions. Simulations were performed for three different initial SO_2 plume concentrations equal to 10 ppb, 100 ppb, and 1 ppm representing low, moderate and high source emission rates. The above concentrations refer to the stage that the plume touches the ground and therefore is already diluted from the flue gas concentrations. Initial values of the input fluxes from the point source, background concentrations and model variables are presented in Table 1. A single source plume in Mercer

Table 1. *Initial plume and background concentrations for the case studies studying new sulfate particle formation*

Species	Background concentrations (ppb)[a]	Inital concentrations (ppb)		
		weak	moderate	strong
SO_2	10	10	100	1000
NO	0.3	5	50	500
NO_2	3.0	0.28	0.28	0.28
CO	500	210	210	210
ETH	1.5	0.35	0.35	0.35
PAR	150	40	40	40
OLE	0.5	0.025	0.025	0.025
ALD2	8	1.5	1.5	1.5
O_3	130	76.9	76.9	76.9
OH	0.0002	0.004	0.004	0.004

[a] Background concentrations vary with the downwind distance. Representative values are shown here.

County, New Jersey is simulated for 7 July 1988, with the simulation starting at 8:00 a.m. This source was the second largest NO_x emitter in New Jersey; it was also a major CO source. The ambient pollutant concentrations were obtained from a UAM-IV simulation (Morris and Myers, 1990) for the Philadelphia/New Jersey modeling domain (Georgopoulos, 1995), the ambient temperature was 298 K and the initial O_3 concentration was 77 ppb. The production of new particles is known to be strongly influenced by the gaseous concentration of SO_2 and the OH radicals (Kerminen and Wexler, 1996; Lazaridis et al., 1997). The simulations were performed with initial SO_2 to NO content ratio equal to 2:1.

Fig. 1 presents the nucleation rate (particles/ m^3 s) at the plume centerline versus plume travel time for the three different emission scenarios. Higher SO_2 emissions lead to higher production of sulfate particles compared to the moderate and low emission scenarios. Therefore, controlling SO_2 emissions also reduces the potential for new sulfate particle formation. In the early stages of plume transport there is no significant formation of new particles due to low concentrations of OH radicals. This is due to high NO concentrations which result in lowering the O_3 concentration (primary source for OH). In later stages of transport the plume is further dilute and there is strong production of OH due to nonlinear chemical reactions and entrainment from the background air. Eventually, the plume reaches background levels of SO_2 but it still has a high OH concentration which results to higher productions of sulfate particles compared to background conditions.

Observations of Hegg et al. (1985) at strong SO_2 point sources show a concentration of submicron particles close to 10^{12} particles/m^3. However, no direct comparison can be performed against the experimental data since the particle number concentration is changing dynamically in a plume that constantly dilues.

Fig. 2 shows the nucleation rate (particles /m^3 s) versus plume evolution time (min) for different cells along the plume cross-section for the case of high initial SO_2 concentrations (1 ppm). The homogeneous nucleation rate of the sulfuric acid - water system is higher close to the plume centerline but nucleation in outer cells starts at earliest stages of the plume evolution. This is due to higher initial OH concentrations at the edge of the plume and is in agreement with the findings of Kerminen and Wexler, (1996), where higher nucleation rates were predicted at the edge of the plumes during the first minutes of plume dispersion. Both studies show that the nucleation rate is stronger close to the plume centerline.

The OH concentration is higher in the outer

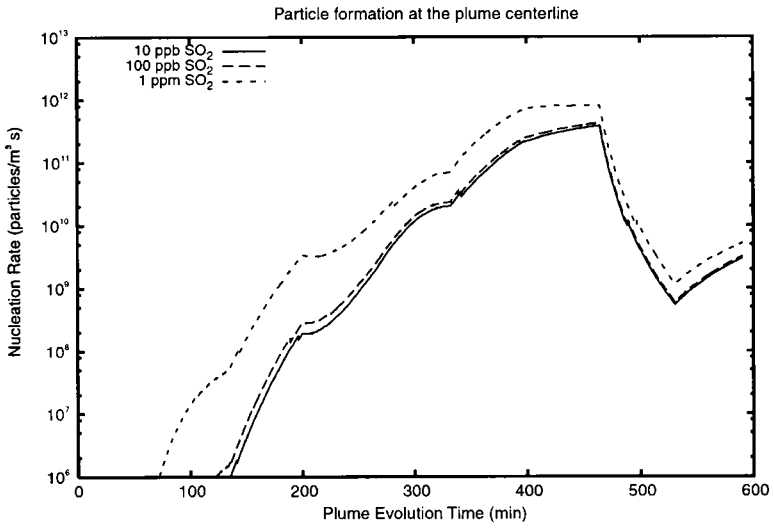

Fig. 1. Nucleation rate (particles/ m^3 s) versus transport time (minutes) of plume for different initial SO_2 concentrations corresponding to low (10 ppb), moderate (100 ppb) and high (1 ppm) sources.

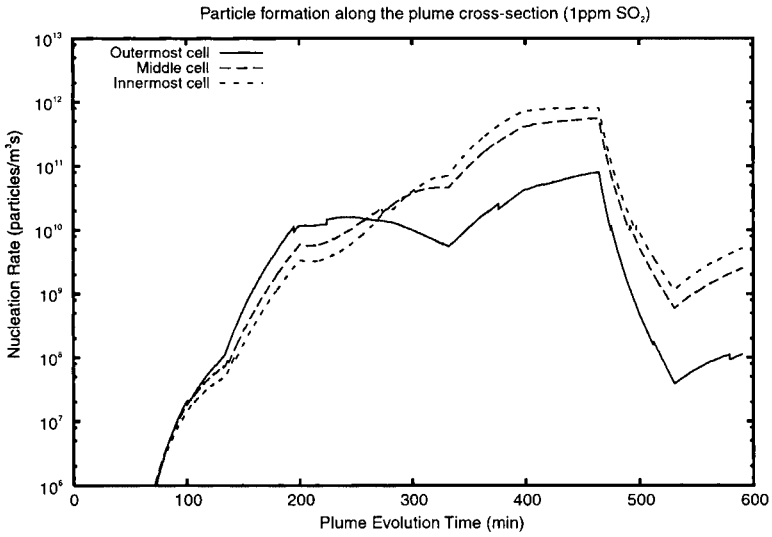

Fig. 2. Cross section nucleation rate at different plume travel times for high initial SO_2 concentration (1 ppm).

cells at earlier times of plume dispersion and therefore nucleation first occurs in the outer cells of the plume. However, OH concentrations in the outer cells decline faster compared to levels in the inner cells, due to air entrainment from outside the plume, and therefore nucleation rates are slowing down (see also Fig. 2). Maximum OH concentrations for the inner cells occur later than for outer cells due to high NO concentrations at the early stages of plume transport. Furthermore, SO_2 concentration is decreasing drastically during the first hour of transport due to plume expansion and eventually the plume SO_2 levels are approaching background values for all the cells.

The simulations show that nucleation of sulfur particles in plumes is a favorable process which leads to a high number of nanometer-size particles. Higher SO_2 emission rates result to higher production of new particles. However, at initial stages of plume dispersion, nucleation is low due to OH depletion by NO. Eventhough high nucleation rates were observed during plume dispersion, the nucleation mechanism is not an important process for mass transfer from the gaseous to particulate phase but it is an important process for new particle formation. The condensation mechanism is the main mechanism for mass transfer from the gaseous to particulate phase (Lazaridis and Koutrakis, 1997). However, a significant increase in the number concentration of the aerosol particle size distribution may have important consequences for cloud formation and indirect climate forcing processes.

3.2. *Comparison with field studies*

The model is also compared with field data from a power plant plumes in Mohave (Nevada) and Navajo (Arizona). Emission data for SO_2, NO_x and particulate matter as well as meteorological data were similar to the data presented by Hudischewskyj and Seigneur (1989). Comparison between model predictions and field measurements for 27 August are shown in Table 2. Available measurements performed at 5.5 Km downwind from the plant shows that the majority of the mass is composed of primary aerosols and only a small amount of sulfate (0.53 $\mu g/m^3$) was present. The field study was performed at 28 August 1979.

Comparison between model predictions and field data for the 28, 31 August 1979 and 11 August 1980 are also shown in Tables 3–5. Comparisons between the model predictions and the measurements are quite satisfactory for SO_2, NO, NO_2 and O_3. For sulfate the model underestimates the mass concentration near the source but overestimates it at larger distances downwind the source. The reason is probable due to presence of aged air masses that are mixed with the polluted plume and uncertaincies in primary emissions of

Table 2. *Comparison of measured and calculated plume concentrations for the Mohave power plant plume in Nevada (27 August 1979)*

Species	Measured	Predicted
5.25 km from the source		
SO_2	0.73 ppm	0.825 ppm
NO	0.75 ppm	0.54 ppm
NO_2	0.07 ppm	0.11 ppm
O_3	0	4.93×10^{-3} ppm
SO_4^{2-}	0.92 μg m^{-3}	0.26 μg m^{-3}
27.8 km from the source		
SO_2	0.15 ppm	0.1 ppm
NO	0.09 ppm	0.02 ppm
NO_2	0.35 ppm	0.03 ppm
O_3	0.01 ppm	0.065 ppm
SO_4^{2-}	0.36 μg m^{-3}	0.76 μg m^{-3}

Table 3. *Comparison of measured and calculated plume concentrations for the Mohave power plant plume in Nevada (28 August 1979)*

Species	Measured	Predicted
5.5 km from the source		
SO_2	0.56 ppm	0.32 ppm
NO	0.62 ppm	0.13 ppm
NO_2	0.35 ppm	4.0×10^{-2} ppm
O_3	0	5.0×10^{-2} ppm
SO_4^{2-}	0.69 μg m^{-3}	0.11 μg m^{-3}
55.5 km from the source		
SO_2	0.03 ppm	0.03 ppm
NO	0.02 ppm	0.038 ppm
NO_2	0.04 ppm	0.013 ppm
O_3	0.02 ppm	0.06 ppm
SO_4^{2-}	0.2 μg m^{-3}	0.53 μg m^{-3}

particulate matter. However, the results for sulfate mass are quite reasonable and in qualitative agreement with the field studies. Another possible reason for the discrepancies between the modelling results and the measured concentrations may connected with presence of yet poorly-qualified heterogeneous formation pathways for secondary sulfate as indicated by Rodhe (1999) and Roelofs et al. (1998).

The 3 modelled cases for 1979 show substantially lower values for NO_2 than the measured values. Hegg et al. (1985) noticed also these high values for NO_2 and they pressumed an error in the measurements or high emissions due to chronic operational problems from the stack itself.

Table 4. *Comparison of measured and calculated plume concentrations for the Mohave power plant plume in Nevada (31 August 1979)*

Species	Measured	Predicted
5.5 km from the source		
SO_2	0.34 ppm	0.47 ppm
NO	0.42 ppm	0.3 ppm
NO_2	0.3 ppm	0.14 ppm
O_3	0.01	0.08 ppm
SO_4^{2-}	1.19 μg m^{-3}	0.13 μg m^{-3}
25.9 km from the source		
SO_2	0.03 ppm	0.12 ppm
NO	NA ppm	3.8×10^{-2} ppm
NO_2	0.04–0.05 ppm	0.05 ppm
O_3	0.05 ppm	0.027 ppm
SO_4^{2-}	0.71 μg m^{-3}	0.52 μg m^{-3}

Table 5. *Comparison of measured and calculated plume concentrations for the Mohave power plant plume in Nevada (11 August 1980)*

Species	Measured	Predicted
5.5 km from the source		
SO_2	0.64 ppm	0.69 ppm
NO	0.47 ppm	0.42 ppm
NO_2	0.05 ppm	0.08 ppm
O_3	0	3.6×10^{-3} ppm
SO_4^{2-}	3.25 μg m^{-3}	0.2 μg m^{-3}

Hudischewskyj and Seigneur (1989) predicted also much lower NO_2 concentrations than the measured ones. However, for the 1980 measurements the predicted values are quite close to the measured data.

Furthermore, the model is applied to study plume concentrations in the Navajo power plant. Table 7 shows the predicted values against meas-

Table 6. *Comparison of measured and calculated plume concentrations for the Navajo power plant plume (13 July 1979)*

Species	Measured	Predicted
5.5 km from the source		
SO_2	0.08 ppm	0.071 ppm
NO	0.02 ppm	0.037 ppm
NO_2	0.02 ppm	0.019 ppm
O_3	0.04	0.039 ppm
SO_4^{2-}	0.23 μg m^{-3}	0.7 μg m^{-3}

Table 7. *NMVOC speciation used in the emission scenario; % by mass allocated to each species*

Species	Vehicle	Oil sector			
		loading buoys	flare	turbine	transport
C_2H_6	4.86	34	12.50	18.75	5.7
C_4H_10	30.87	66	12.50	25.00	18.0
C_2H_4	8.63		6.25	12.50	12.0
C_3H_6	7.00		18.75	12.50	4.6
C_8H_10	36.76		37.50	25.00	10.6
HCHO	1.64		7.50	3.75	5.9
CH_3CHO	1.06		5.00	2.50	4.0
CH_3OH	0.0				
C_2H_5OH	8.75				39.2

ured data for various gaseous species and sulfate aerosols. In this case the model overpredicts the sulfate concentration by a factor of 3. Possible explanations can be uncertainties in the primary aerosol emissions which are difficult to estimate.

The plume model has the capability of simulating also the chemical composition of the aerosol size distribution but for that an extensive set of measured data are necessary such as speciated emissions of primary particles and background aerosol concentrations. In the current comparisons the model was in reasonable quantitative agreement with the available field data.

3.3. Condensible organic carbon (COC) production from different emission sources

The condensible organic compound (COC) yields method for the lumped organic compounds (Pandis et al., 1992) is applied here to study secondary organic aerosol formation in plumes. Two hypothetical scenario using representative emissions from vehicles and activities in the oil sector were modelled. A hypothetical emission of 0.3 ppm NMVOC is used and this amount is speciated according to the Table 7 (EMEP, 1996). The hypothetical emissions from vehicles and oil activities were modelled as point sources. The present simulations have as a primary objective to study a hypothetical evolution of the gaseous and aerosol organic components arising from emissions from vehicles and the oil sector. The inherent interest in this study is the evaluation of the secondary organic matter potential of the above mentioned sources. It is clear that vehicle emissions in principle cannot be viewed spatially as a point source. However, the reason for this assumption is due to the fact that we are mainly interested in the differences associated with the production of secondary organic aerosols from different types of sources.

Fig. 3 presents the evolution of the organic particulate matter production during a hypothetical emission scenario from the oil sector. Model results show that secondary organic aerosol formation contributes in the aerosol concentration but is much lower than the sulfate production rates originitating from major sulfur sources (see Tables 2–6). The modified CB-IV chemical mechanism (Lurmann et al., 1997) has been used in the above simulations. In Fig. 4 we plot the evolution of average gaseous concentrations of the NMVOC species as well as the concentrations of ozone, NO, NO_2, SO_2 and OH in the plume. Dilution due to entrainment of background air in the plume results to a considerable reduction in the concentration of the emitted gaseous species.

Fig. 5 shows the differences in the COC production from two hypothetical emission scenario of 0.3 ppm NMVOC speciated according to Table 7. Vehicle emissions have a considerable higher potential for COC production compared to the oil sector. This is mainly due to higher percentage of the highly reactive o-xylene in the vehicle emissions and the high alkane emission characteristics of the oil sector.

The use of the COC formation capability in the chemistry module (CB-IV mechanism) of the plume model is an important step which enhances our capability in estimating the aerosol concentration/chemical composition in plumes. However, the partitioning of organic matter in the atmosphere is highly uncertain due to great complexity of the number of different chemical forms of organic matter and the absence of direct chemical analysis.

4. Conclusions

In summary, a number of different conclusions were reached with the use and application of the current aerosol plume model. In general, the plume model is an efficient modeling platform for

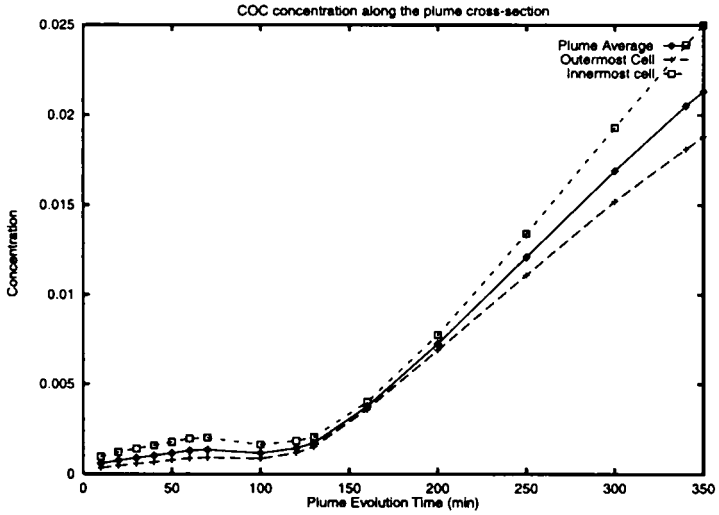

Fig. 3. Production of COC ($\mu g/m^3$) during typical emissions from the oil sector along the plume cross-section.

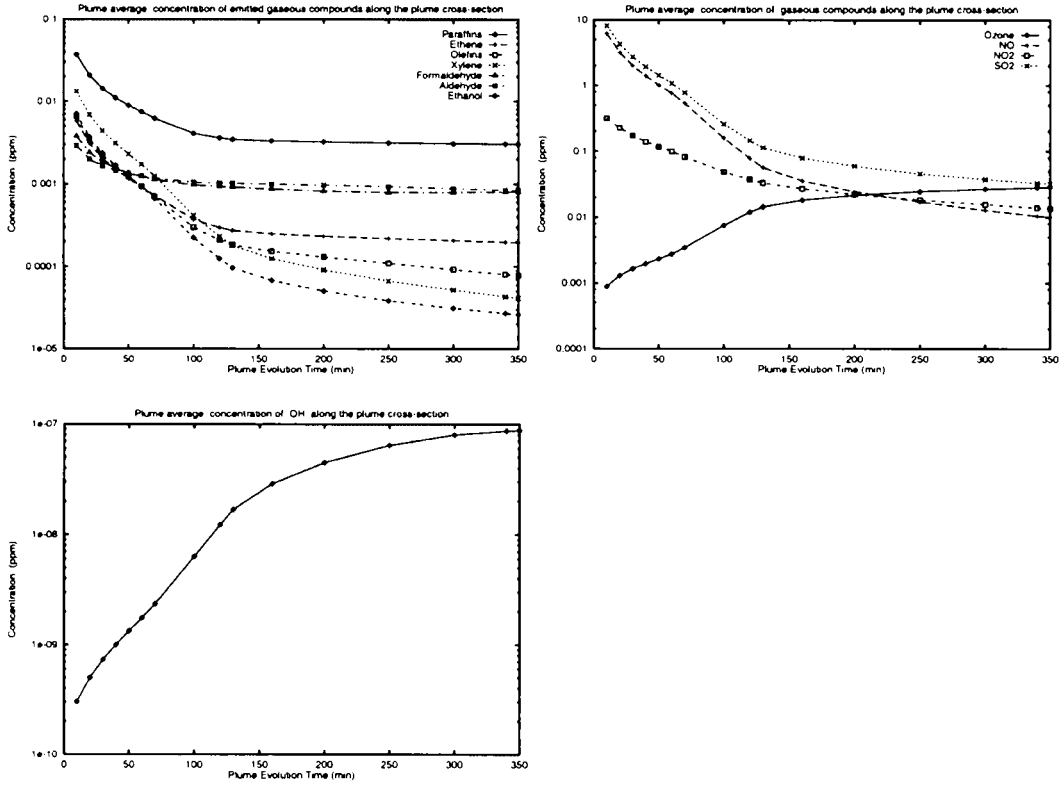

Fig. 4. Average ambient concentration of (a) various organic emitted gaseous components from the oil sector; (b) ozone, NO, NO_2 and SO_2; (c) OH.

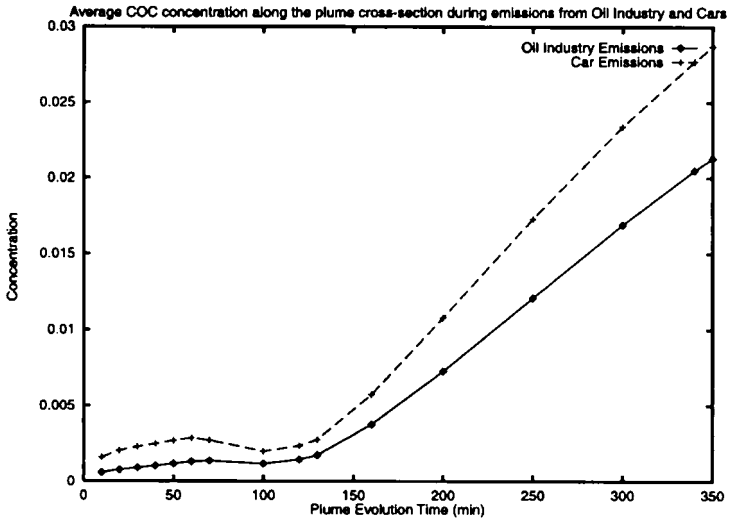

Fig. 5. Differences in the COC production potential ($\mu g/m^3$) due to emissions from vehicle and oil industry emissions.

performing aerosol and gaseous species calculations and is checked against several field data.

The plume model is applied first to study new sulfate particle formation from plumes emitting high SO_2 concentrations. A high number of subnanometer sulfate aerosols is formed during the plume evolution of SO_2 from point sources, where higher nucleation rates are predicted close to the plume centerline and for higher SO_2 emission rates. At the initial stages of plume transport nucleation occurs only in the outer cells of the plume due to OH depletion by NO in the inner cells. Therefore, controlling SO_2 emissions also reduces the potential for new sulfate particle formation, The current simulations are in qualitative agreement with the experimental observations of Hegg et al. (1985) for strong SO_2 point sources, where a concentration of submicron particles close to 10^{12} particles/m^3 was observed.

Furthermore, the plume model is compared with field data from two power plants in the USA. The model calculations are in satisfactory agreement with field measurements in several power plant plumes for SO_2, NO, NO_2, O_3 and sulfate particles.

Finally, the model is applied to study the formation of COC from vehicle sources and activities in the oil sector performing two example scenario using realistic non-methane volatile organic compounds (NMVOC) emission speciation. Vehicle emissions are expected to have a higher potential for secondary organic matter formation based on the current simulations.

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