COVER SHEET

A Review of Dispersion Modelling and its application to the dispersion of particles: An overview of different dispersion models available.

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Abstract

This paper provides the first review of the application of atmospheric models for particle dispersion. The different types of dispersion models available, from simple box type models to complex fluid dynamics models are outlined and the suitability of the different approaches to dispersion modelling within different environments, in regards to scale, complexity of the environment and concentration parameters is assessed. Finally, several major commercial and non-commercial particle dispersion packages are reviewed, detailing which processes are included and advantages and limitations of their use to modelling particle dispersion. The models reviewed included: Box models (AURORA, CPB and PBM), Gaussian models (CALINE4, HIWAY2, CAR-FMI, OSPM, CALPUFF, AEROPOL, AERMOD, UK-ADMS and SCREEN3), Lagrangian/Eulerian Models (GRAL, TAPM, ARIA Regional), CFD models (ARIA Local, MISKAM, MICRO-CALGRID) and models which include aerosol dynamics (GATOR, MONO32, UHMA, CIT, AERO, RPM, AEROFOR2, URM-1ATM, MADRID, CALGRID and UNI-AERO).

Table of Acronyms used

Models

AERMOD	American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee Dispersion Model)
AEROFOR2	Model for Aerosol formation and Dynamics
AURORA	Air Quality Modelling in Urban Regions using an Optimal Resolution Approach

CACM	Caltech Atmospheric Chemistry Mechanism
CALGRID	California Photochemical grid Model
CALINE4	California Line Source Dispersion Model
CALPUFF	California Puff Model
CAQM	Community multiscale air quality model.
CAR-FMI	Contaminants in the Air from a Road – Finnish Meteorological Institute
CBM-IV	Chemical Bond Mechanism Version IV
CIT	California/Carnegie-Mellon Institute of Technology
CMEM	Comprehensive Modal Emission Model
CPB	Canyon Plume Box
EQSAM	Equilibrium Simplified Aerosol Model
GATOR	Gas Aerosol Transport Radiation Model
GRAL	Graz Lagrangian Model
ISORROPIA	Thermodynamics “Equilibrium” Model (from the greek word)
MADRID	Model of Aerosol Dynamics, Reaction, Ionization and Dissolution
MEASURE	Mobile Emissions Assessment System for Urban and Regional Evaluation
MICRO-CALGRID	Microscale California Photochemical grid Model
MISKAM	Microscale flow and dispersion model
MONO32	Multimono
OSPM	Operational Street Pollution Model
PBM	Photochemical Box Model
RACM	Regional Atmospheric Chemistry

RADM	Regional Acid Deposition Mechanism
RPM	Regional Particulate Model
SAPRC	Statewide Air Pollution Research Center
SCREEN3	Screening version of ISC3 model
SEQUILIB	Sectional Equilibrium Model
STAR-CD	Simulation of turbulent flow in arbitrary regions Computational Dynamics
TAPM	The Air Pollution Model
TREFIC	Traffic Emission Factor Improved Calculation
UAM IV	Urban Airshed Model with Aerosols Version 4
UAM-AERO	Urban Airshed Model with Aerosols
UHMA	University of Helsinki Multicomponent Aerosol Model
UK-ADMS	UK Atmospheric Dispersion Modeling System
UNI-AERO	EMEP Aerosol Dynamics Model
URM-1ATM	Urban-Regional Model
Other terms	
CBL	Convective boundary layer
CERC	Cambridge Environmental Research Consultants
CFD	Computational Fluid Dynamic
CMU	Carnegie-Mellon University
EMEP	Co-operative Programme for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe
FA2	Fraction of modelled values within a factor of 2 of measured values
GRS	Generic reaction set

NMSE	Normalised mean square error
PM_{10}, $PM_{2.5}$, PM_x	Particulate matter in the atmosphere with an aerodynamic diameter less than 10, 2.5 μm or some value x.
SOA	Secondary Organic Aerosol
UK	United Kingdom
uv	ultraviolet
ZSR	Zdanovskii Stokes Robinson

1. Introduction

Dispersion modelling uses mathematical equations, describing the atmosphere, dispersion and chemical and physical processes within the plume, to calculate concentrations at various locations. Whilst, there have been various review papers on atmospheric modelling and their approaches to dispersion in street canyons(Vardoulakis, Fisher et al. 2003) and comparisons between different models using test meteorological data(Ellis, McHugh et al. 2001; Sivacoumar and Thanasekaran 2001; Hall, Spanton et al. 2002; Caputo, Gimenez et al. 2003), these have focussed on modelling gaseous dispersion.

Unfortunately, only a few studies have simultaneously measured particle concentration with gases and the differences between the studies may be partially responsible for the differences observed. In open sites several studies have shown varying correlations between the concentrations of gases and particles. Monn et al. (1997) (Monn, Fuchs et al. 1997) showed a poor correlation between the outdoor PM_{10} concentrations and NO_2 concentrations in an urban environment with a better correlation between $PM_{2.5}$ and NO_2, although only 2 locations were studied in the latter case. In contrast, Clairborn (1995) (Clairborn, Mitra et al. 1995) showed a good

correlation between SF_6 and PM_{10} although only distances upto 60m from the motorway were measured. Roorda-Knape et al. (1998) (Roorda-Knape, Janssen et al. 1998) observed that benzene, $PM_{2.5}$ and PM_{10} showed no significant decrease in concentration upto 300m from a major motorway. This was consistent with the small decrease in the $PM_{2.5}$ concentration observed by Hitchins et al. (2000)(Hitchins, Morawska et al. 2000). In that study the authors observed that particle number concentration decreased faster than NO_2 concentration from a motorway. Zhu et al. (2002)(Zhu, Hinds et al. 2002a; Zhu, Hinds et al. 2002b) showed that number concentration of particles between 6 and 220nm correlated well with CO concentration from a motorway. All of these studies were made in an open environment where the wind direction was perpendicularly away from the road. However, differences have been observed between the local dispersion of gases and particles(Morawska 2003; Holmes, Morawska et al. 2005). Simultaneous measurements of CO and particle number concentration showed that CO concentration was not significantly correlated to particle number concentration around the site and examination of between-site comparisons with the two pollutants showed different spatial and temporal trends. In another study of urban sites Harrison and Jones (2005) (Harrison and Jones 2005), observed that particle concentrations correlated only weakly with NO_x, with the highest correlation observed at a curbside monitoring location, where concentrations are less affected by dispersion. In addition, an examination of many urban studies(Morawska 2003) has shown that the vertical profiles of particle number concentration around buildings differed from that of gases. These studies differ from the previous studies in that they were conducted in a more complex environment where wind flows were heavily affected by turbulence and emissions were not limited to a single line source. In general the studies show that in

open environments the gas and particle concentrations correlate quite well, whilst in a more complex urban environment significant differences are observed between gas and particle dispersion. In an urban environment where traffic emissions are the dominant source of particles particle Van Dingenen et al. (2004)(Van Dingenen, Raes et al. 2004) showed $PM_{2.5}$ and PM_{10} had an R^2 value of 0.95 across all sites in the monitoring network. However, the $PM_{10}/PM_{2.5}$ ratio varied too much to propose a single $PM_{10}/PM_{2.5}$ ratio. In the same study they observed no correlation between annual average particle number concentration and either $PM_{2.5}$ or PM_{10} concentrations. This is in contrast to Harrison et al. (1999) (Harrison, Jones et al. 1999) who found that in an urban measurement study hourly particle number concentration more closely correlated with $PM_{2.5}$ than PM_{10} measurements, although both PM ranges showed good correlation with the hourly particle number concentrations during the 3 month period.

Therefore, models that are designed to model the dispersion of passive scalars, such as inert gases should be capable of modelling the $PM_{2.5}$ and PM_{10} concentrations in certain open environments, especially for longer averaging periods and in the larger airshed where short term variations resulting from transient particle formation events are evened out.

The modelling of particle number concentration involves the incorporation of aerosol dynamics modules into dispersion models. Thus the discussion of particle dispersion modelling must involve both a discussion of the limitations of the various dispersion approaches to the treatment of particles and the aerosol dynamic packages used to evaluate particle processes occurring within the plumes. To complicate the situation further, Lohmeyer (2001) (Lohmeyer 2001)observed that concentrations calculated by the different models differed by a factor of four and even when the same model was

employed results varied between groups. The agreement with predicted concentrations was seen to depend on the quality of the input data.

This review will outline the different model types, looking at specific requirements for the different spatial scales from local to regional models, and deficiencies with respect to particle dispersion and aerosol dynamics within different scales. In addition, whilst not being a comprehensive review of all models available a large number of models are included in the review and the more important model parameters and inputs for the models are listed in Tables 1a and b and Table 2.

Although several models claim to be able to model particle dispersion, without specific treatment of particle dynamics the results are limited to calculation of particle mass, usually in the form of $PM_{2.5}$ and PM_{10}, and cannot calculate particle number concentration.

Furthermore particle validation studies are not available for many models. Where this is the case the authors have attempted to highlight model performance in terms of gas dispersion validation studies. Since several studies have shown a good correlation between non reactive gases and particles within a larger airshed, validation studies involving gases should be a good indicator of the performance of the model in terms of calculating particle mass concentrations, as discussed earlier. In addition, different averaging times between average gas and particle concentrations make comparison difficult and mean that it is often impossible to determine whether changes between gas and particle concentrations predicted by the model correlate so well.

A number of local and regional models exist that include extensive treatment of aerosol dynamics. The majority of these are non commercial packages and have been coupled to existing dispersion models in order to provide a package that is able to model changes to particle number concentration within different size groups. This

means that the performance of these models depends on both the accuracy and specific processes included in the dynamics module as well as the performance of the dispersion model. It is often possible to integrate the aerosol dynamics module with different dispersion models to adapt the coupled dispersion package to better suit the planned study.

2. Modelling Methodology

2.1. Box Models

Box models are based on the conservation of mass. The site is treated as a box into which pollutants are emitted and undergo chemical and physical processes. It requires the input of simple meteorology and emissions and the movement of pollutants in and out of the box is allowed. The inside of the box is not defined and the air mass is treated as if it is well mixed and concentrations uniform throughout. One advantage of the box model is because of the simplified meteorology box models can include more detailed chemical reaction schemes (e.g. Master Chemical Mechanism) and detailed treatment of the aerosol dynamics, that are able to represent the chemistry and physics of particles within the atmosphere better. However, following inputting initial conditions a box model simulates the formation of pollutants within the box without providing any information on the local concentrations of the pollutants. For this reason they are unsuitable to modelling the particle concentrations within a local environment, where concentrations and thus particle dynamics are highly influenced by local changes to the wind field and emissions.

2.2. Gaussian Models

Gaussian type models are widely used in atmospheric dispersion modelling, in particular for regulatory purposes, and are often "nested" within Lagrangian and Eulerian models. Gaussian models are based on a Gaussian distribution of the plume in the vertical and horizontal directions under steady state conditions. The normal distribution of the plume is modified at greater distances due to the effects of turbulent reflection from the surface of the earth and at the boundary layer when the mixing height is low. The width of the plume is determined by σ_y and σ_z, which are defined either by stability classes(Pasquill 1961; Gifford Jr. 1976) or travel time from the source. One severe limitation of plume models with regards to modelling particle dispersion is that since the plume models use steady state approximations they do not take into account the time required for the pollutant to travel to the receptor. Therefore, aerosol dynamics must be calculated by post processing treatment of the results. In addition, regional modelling generally requires the incorporation of chemical modelling to accurately predict the formation of particles through secondary organic aerosol (SOA) formation. Even NO_x and SO_x chemistry, which is fundamental to determining particles and ozone concentrations, is often only calculated using a simple exponential decay. More advanced models can simulate some of the chemical transformations using post processing treatment of the chemistry. Although most Gaussian models only consider diffusion and advection of the pollutants more advance Gaussian models have recently been developed that include physical processes such as deposition and fast chemical reactions. Furthermore, the Gaussian plume equation assumes that there is no interaction between plumes, which can become significant within urban environments.

Algorithms have been developed to model the chemistry and physical processes within the plume and dispersion around buildings. The effect of wakes from buildings can be achieved by modifying the dispersion coefficients, σ_y and σ_z. However, the Gaussian equation is not able to calculate recirculation effects caused by multiple buildings or at intersections.

Some of the restrictions implicit in the Gaussian Plume models can be overcome by approximating the emission as a series of puffs over time, which allows the wind speed to be varied. In this approach each puff behaves according to the Gaussian dispersion equation and the overall contribution of the source is calculated by integration of the individual puffs with respect to time and summation of the contribution of individual puffs at the receptor position.

In order to calculate the concentration of pollutants over an urban area multiple source plumes are often used. The different equations used are determined by the nature of the source and heights of the source and receptor.

Some further limitations of the Gaussian treatment means that Gaussian models are not designed to model the dispersion under low wind conditions or at sites close to the source, *i.e.* distances less than 100m. Gaussian models have been shown to consistently overpredict concentrations in low wind conditions(Benson 1984; Sokhi, Fisher et al. 1998). Hybrid models, which use a combination of the Gaussian plume and puff models, include along wind dispersion of the pollutants in order to better estimate concentrations under low wind speed conditions(Sharan, Yadav et al. 1996; Thomson and Manning 2001). A further limitation is a result of the simplified treatment of turbulence and meteorology so they are best suited to calculating hourly pollutant concentrations.

Since Gaussian plume equations assume a homogeneous wind field it is not recommended that they are used for far field modelling as the meteorology is expected to change over such large distances. Caputo et al. (2003)(Caputo, Gimenez et al. 2003) observed that four Gaussian models calculated non zero concentrations for the whole downwind domain and so suggested that they should be limited to distances a few tens of kilometres from the source.

2.3. Lagrangian Models

Lagrangian models are similar to box models in that they define a region of air as a box containing an initial concentration of pollutants. The Lagrangian model then follows the trajectory of the box as it moves downwind. The concentration is a product of a source term and a probability density function as the pollutant moves from x to x'.

Lagrangian models incorporate changes in concentration due to mean fluid velocity, turbulence of the wind components and molecular diffusion.

Lagrangian models work well both for homogeneous and stationary conditions over the flat terrain(Oettl, Kukkonen et al. 2001; Raza, Avila et al. 2001; Venkatesan, Mathiyarasu et al. 2002; Tsuang 2003) and for inhomogeneous and unstable media condition for the complex terrain(Du 2001; Hurley, Manins et al. 2003; Jung, Park et al. 2003). It is possible to model the non-linear chemistry using either the superimposition of a concentration grid on the domain, followed by calculation of the concentration in each grid or the particle can be treated as an expanded box and the photochemical module of the model applied to each box.

The meteorological data calculates the variance of the wind velocity fluctuations and Lagrangian autocorrelation function. Since Lagrangian particle models calculate the

diffusion characteristics by the generation of semi random numbers they are not confined by stability classes or sigma curves, as is the case with Gaussian dispersion models.

2.4. Computational Fluid Dynamic Models

Computational fluid dynamic (CFD) models provide complex analysis of fluid flow based on conservation of mass and momentum by resolving the Navier-Stokes equation using finite difference and finite volume methods in three dimensions. Turbulence is classically calculated using k-ε closure methods to calculate the isotropic eddy viscosity parameter present in both the momentum and pollution transport equations, which assumes that a pollutant is diluted equally in all directions. This treatment performs well on a flat boundary layer. However, when a stratified boundary layer exists the closure method needs to be modified to include the Coriolis force and reduced wind shear in the upper atmosphere, which results in an overestimation of the eddy viscosity.

Gidhagen et al. (2004)(Gidhagen, Johansson et al. 2004) reported that different CFD models showed good agreement in overall wind flow field but demonstrated that although the inputs were identical the models gave large differences in velocities and turbulence levels. Comparison with the wind tunnel data suggested that this was a result of the closure mechanisms used by the different models.

3. Overview of models for dispersion within a street environment

A review of urban dispersion models is given by Vardoulakis et al. (2003)(Vardoulakis, Fisher et al. 2003) so only a brief summary of the models will be given here together with a discussion of their applicability to model particle

dispersion. Although there are a number of dispersion models used to calculate urban pollutant concentrations in a local environment, some of which also include a complex treatment of wind flow in street canyon environments, only three models include a module to calculate particle dispersion.

3.1. Models that exclude specific treatment of aerosol dynamics

Dispersion models that do not include a module for chemical formation (nucleation) or aerosol dynamics (coagulation, condensation etc) are not capable of calculating particle number concentration. Since the models are generally based on conservation of mass they are capable of modelling the dispersion of particles, in terms of $PM_{2.5}$ or PM_{10}. The models generally treat the particles in a similar way to gases and as discussed earlier this can be dangerous depending on the averaging period and location. However, since air quality regulations are currently based on particle mass concentrations simple particle dispersion models are essential and so the performance of the most commonly used regulatory models will be discussed as part of this review.

3.1.1. Box models

AURORA (VITO, Belgium) is an integrated air quality model that has been used to model the concentration of inert and reactive gases and particles in an urban environment (Mensink, Colles et al. 2003). The model uses a steady state box model to calculate the pollutant concentrations within a street canyon. The model assumes a uniform concentration over the street but includes turbulent intermittency in the flow from the upwind roof of the canyon. Inside the box both convection in the x and z directions are considered.

The CPB (GEOMET) is an urban canyon box model that has been designed for urban canyons with height to width ratios between 0.5 and 2. The model calculates the average concentration of inert gases and NO_2, using a simple algorithm for the reaction of NO with ozone, within a street canyon for three different wind flows.

3.1.2. Gaussian Models

Two of the most common models used to calculate the dispersion of vehicle emissions are CALINE4 (California Department of Transportation) and HIWAY2 (US EPA). Both models are based on a Gaussian plume model and so suffer from the inherent limitations of the Gaussian equations to urban dispersion modelling over short distances and within complex environments. In addition, their use is not recommended for the modelling in low wind speeds. Despite these problems they have been applied in a large number of studies and for regulatory purposes due to their ease of use and since they do not require extensive computer power or time.

Both models treat traffic as an infinite line source divided into a series of elements located perpendicular to the wind direction. Vertical dispersion parameters in CALINE 4 take into consideration both thermal and mechanical turbulence caused by vehicles, whilst HIWAY 2 only considers the effects of vehicles and ignores the effect of thermal turbulence on vertical dispersion. In addition to the problems stated above, Gaussian models (*e.g.* CALINE4 AND HIWAY2) lack the sophistication required for modelling in street canyons as buildings can only be represented by changing the surface roughness.

CAR-FMI (Finnish Meteorological Institute) is a Gaussian Plume model based on the equations of Luhar and Patil (1989)(Luhar and Patil 1989). It is designed to calculate

the hourly concentrations of CO, NO, NO_2, NO_x and $PM_{2.5}$ from vehicles. Atmospheric stability is defined using Boundary layer scaling. As with the other Gaussian models CAR-FMI is limited in its use in low wind conditions. The horizontal and vertical dispersion parameters (σ_y and σ_z) included turbulence terms from ambient wind speed, exhaust velocities and vehicles.

As with CALINE4, CAR-FMI models the dispersion of inert and reactive gases and PM, using the discrete parcel method. However, unlike CALINE4 it contains treatment of dry deposition for 3 particle size groups. Oettl et al. (2001)(Oettl, Kukkonen et al. 2001) demonstrated that hourly NO_x concentrations measured at a major road in Finland agreed fairly well with model predictions by CAR-FMI and GRAL. However, CAR-FMI was not able to predict the meandering wind flow under low wind speed conditions.

OSPM is a semi empirical model that uses a Gaussian plume equation to derive the direct contribution from the source and a box model to calculate the effect of turbulence on the concentrations(Vignati, Berkowicz et al. 1999). Cross wind diffusion within the plume is disregarded and the sources are treated as infinite line sources. The plume expression for a line source is integrated along the path defined by the street level wind.

The wind direction at the street level is assumed to be mirror reflected with respect to the roof level wind. The wind speed at street level is calculated from the synoptic wind speed and direction and surface roughness. The treatment and contribution of the various turbulent processes within the street canyon vary depending on the synoptic wind speed and direction and the reader is directed to Vignati et al. (1999)(Vignati, Berkowicz et al. 1999) for a full description. The model allows for effects of the

turbulence on the concentrations at the windward and leeward sides of the canyon by neglecting the direct component of the emissions for the windward side of the street.

The model assumes that the traffic emissions are uniformly distributed across the canyon and empirically derives the effect of vehicle induced turbulence. The simple treatment of turbulence means that the model is unable to model the intermittent fluctuations of wind flow and is therefore not recommended for calculating concentrations on timescales shorter than one hour. Additionally the model does not take into account the cooling of the exhaust plume after emission, which could have a significant effect on the formation of SOA particles.

The OSPM model was evaluated against measured data in an urban street canyon(Kukkonen, Partenan et al. 2003) for NO_x, NO_2, O_3 and CO. Predicted hourly averaged concentrations showed fairly good agreement both at roof top and street level. Whilst the correlation showed that it was possible to predict hourly concentrations using modelled background concentrations and pre processed meteorological data, no attempt was made to predict concentrations for shorter time periods.

In a second study(Ketzel, Berkowicz et al. 2000) the agreement of OSPM with street values was not as good and failed to accurately predict the effect of different wind directions on hourly NO_2 concentrations in two street canyons. However, it did accurately calculate the contribution of vehicle traffic to the annual benzene concentration at street level. This underlines the inability of the simplified treatment of wind flow within the canyon to reflect short term changes in concentration.

3.1.3. Lagrangian (and Eulerian) Models

GRAL (Institute for Internal Combustion Engines and Thermodynamics, Graz, Austria) is a coupled Eulerain-Lagrangian Model designed to model the dispersion of inert compounds within inhomogeneous wind fields. One limitation is that the model can not take into account any chemical formation of particles (e.g. ammonium nitrates, ammonium sulfates). The model calculates concentrations from 10 minutes upto 1 hour for line and point sources as well as from tunnel portals within flat(Oettl, Sturm et al. 2005) and complex terrain(Oettl, Sturm et al. 2003). The atmospheric stability is calculated using boundary layer scaling. The model assumes a constant plume rise in the vicinity of the tunnel portal as a function of the temperature difference between the ambient air and the tunnel flow.

No validation studies currently exist for the use of GRAL with particles, although the designers are currently involved with performing quite intensive simulations for PM_{10} and $PM_{2.5}$ for cities. However, the model accurately simulated the concentrations of SF_6 during varying wind speeds from four tunnels surrounded by varied topography, although the calculations for all three tunnels are highly influenced by the low concentration values. In particular, the concentration measurements around the Nimomiya tunnel show considerable disagreement(Oettl, Sturm et al. 2003). In a recent study the model accurately predicted the mean hourly NO_x concentration at four locations around an urban tunnel. At the fifth location the model failed to calculate the concentration since this location was heavily affected by surrounding streets not included in the model. Despite the good performance of the model it is not universally applicable without experience, since there are two empirical parameters that are adjusted by the user due to traffic volume and specifics of the tunnel locations, this could be the result of the poor agreement in parts for the Nimomiya study.

3.1.4. Computational Fluid Dynamic Models

ARIA Local is a CFD model that has been used to calculate real time dispersion of gases and particles from buses and trains within urban environments(Moon, Albergel et al. 1997; Albergel and Jasmin 1998). A variable resolution grid can be used, with smallest grid sizes below 1 m, to include around 1 million nodes within the area under study. Although, if topography is important it is recommended that equidistant cell sizes are used for the horizontal grid. Three different turbulence models can be used based on either a k-ε or Rij-ε approach with variable gas or fluid characteristics with the atmospheric stability based on the Pasquill categories. Pollution sources include point, line, area and volume releases with the emission generated either as a continuous or volumic release. In addition, the fluid properties of the gases can be adjusted to allow for either buoyant or dense gases. Although not implicitly included in the model the effects of vehicle induced turbulence can be included by adjustment of the model parameters. Chemical transformations can be modelled using a post processing module.

MISKAM is a microscale dispersion for use in built up urban environments. Typically, the domain used is around 300 x 300 m using 60 non equidistant grid cells in each direction, although a larger domain can be modelled. Buildings are treated as blocks and the model does not allow steep topography or include thermal effects, buoyant releases or chemical reactions. The modelling of neutral and stable atmospheric conditions are possible through the use of a turbulent mixing factor. A comparison of annual mean concentrations of an arbitrary pollutant generated within a

wind tunnel with the model results, in a 1.2 x 1.6 x 0.14 km grid, show an excellent agreement (R^2=0.97) although the agreement decreased if the concentrations within the city centre are included (R^2=0.79) (Balczo, Farago et al. 2005). The model has the ability to use a geometrically progressive grid to allow more refined resolution in certain areas.

MICRO-CALGRID (Stern and Yamartino 2001)is an urban canopy scale photochemical model that uses the flow fields and turbulence generated by the MISKAM model. In addition to the features of MISKAM, described above, MICRO-CALGRID incorporates a traffic induced emissions model, MOBILEV(Fige 1997), and the horizontal and vertical advection and diffusion schemes, a full resistance based parameterisation of dry deposition and chemical reaction schemes, SAPRC and CBM-IV, from CALGRID (discussed later in Section 4.4). In addition, the model allows treatment of vehicle induced turbulence through adjustment of the total kinetic energy of the model cells that is produced by a vehicle as it moves through the air. Although no statistical or graphical evidence is provided, the authors state that the behaviour of TSP was well reproduced by the model.

3.2. Local Aerosol models involving detailed treatment of Aerosol dynamics

GATOR(Jacobson 1997) has the option of using either a moving size or stationary size particle dynamics module coupled to a Eulerian dispersion approach to calculate the dispersion of gases and aerosols in urban(Jacobson 1996) /and meso- scale(Lu, Turco et al. 1997) (Jacobson 2001) environments. New particles are generated through homogeneous nucleation that uses parameterizations for the sulphuric acid and water reaction derived over marine environments (Pandis, Russell et al. 1994) and

a recent parameterisation developed for humidities greater than 60%(Fitzgerald, Hoppel et al. 1998). Coagulation is calculated using a semi-implicit algorithm that includes Brownian diffusion (Fuchs 1964), convective Brownian enhancement(Pruppacher and Klett 1997), gravitational collection(Pruppacher and Klett 1997), turbulent inertial motion and turbulent sheer(Saffmann and Turner 1956). Condensation and evaporation are calculated from the gas-surface equilibrium corrected for the Kelvin effect with the liquid water content of the aerosol predicted by the Zdanovskii, Stokes, Robinson (ZSR) method(Robinson and Stokes 1965), including the effects of aqueous phase dissociation of inorganic and organic species. Only dry deposition is modelled using a resistance type approach (McRae, Goodin et al. 1982; Russell, Winner et al. 1993; Seinfeld and Pandis 1998). In addition, the model calculates the solar irradiance that is vital for the calculation of photodissociation from scattering and absorption curves of the particles and gases.

Pohjola et al. (2003)(Pohjola, Pirjola et al. 2003) and Gidhagen et al. (2004)(Gidhagen, Johansson et al. 2004) recently published studies in which they examined the particle dispersion in an urban city environment. Both studies used the particle dynamic model MONO32 but coupled it with different dispersion models, either a simple plume model OSPM(Vignati, Berkowicz et al. 1999) or a CFD dispersion model STARCD(Gidhagen, Johansson et al. 2004) to calculate the number concentration, size distribution and chemical composition of particles. In a study within a road tunnel Gidhagen et al. (2003)(Gidhagen, Johansson et al. 2003), using STARCD, simulated very well the particle number concentration from vehicle traffic. The results showed excellent agreement with the measured data when velocity based emission factors were used. The agreement decreased when constant vehicle emission

factors were used though the correlation was still good. A further study within a street canyon(Gidhagen, Johansson et al. 2004) using MONO32 accurately calculated the hourly particle concentration of particles between 7 and 450 nm using wind speed and direction measured 10m above the roof tops and temperature and rainfall measurements. These simulations also demonstrated that traffic induced turbulence was important to street level dispersion. No significant difference was observed, with and without the influence of vehicle induced turbulence, at wind speeds greater than 5 m s^{-1}. However, at wind speeds of 2 m s^{-1} the total number concentration decreased by 10000 cm^{-3} as a result of vehicle induced turbulence.

The model was able to calculate the main features of the change of NO_x concentration on both sides of the street with wind direction. Particle concentrations showed good agreement with the measured hourly concentration when traffic induced turbulence and changes in aerosol concentrations due to coagulation and deposition were included.

These studies confirm that MONO32 in conjunction with a CFD model can be used to accurately predict aerosol dynamics of particles emitted from vehicles and shows the improvement in the calculation when velocity based emission factors are used for urban modelling. Recently, several new models capable predicting changes in tailpipe emissions as a result of changes in operation, such as acceleration, or a change in gradient have been developed including MicroFac (US EPA)(Singh, Huber et al. 2003), MEASURE (Georgia Tech), CMEM (UC Riverside) and TREFIC (ARIA Technologies).

Using MONO32, Pohjola et al. (2003)(Pohjola, Pirjola et al. 2003) examined the dispersion of four size sections within 25 seconds after emission. They simulated the effects of the various processes on particle number concentration with and without

dilution of the plume. Neither binary nucleation nor ternary nucleation affected particle number during the timescale of the simulation. When dilution was excluded the particle number concentration decreased by an order of magnitude through the effects of coagulation and increased slightly by condensation. However, when dilution was included in the calculation, coagulation had a negligible effect on total particle number although the number of Aitken nuclei mode particles decreased slightly and condensation was only important when the gas phase concentration of the organic compounds exceeded 10^{10} cm^{-3}.

Korhonen et al. (2004)(Korhonen, Lehtinen et al. 2004) developed a size segregated aerosol dynamics model, UHMA, designed to include treatment of aerosol dynamics with a focus on new particle formation and growth. The particles are size segregated based on the volume of the particle core, which is composed of a mixture of sulphuric acid, water soluble organics and a variety of insoluble components. The particle composition within each size category is identical although particle composition varies between different size groups. The organic fraction of the particles is calculated using a lumped description of the compounds, the properties of which can be adjusted by the user depending on the particular conditions.

Nucleation incorporates both binary (Vehkamaki, Kulmala et al. 2002)and ternary nucleation(Napari, Noppel et al. 2002) depending on the atmospheric ammonia mixing ratio, with binary nucleation scheme used for ammonia concentrations lower than 0.1 ppt.

Growth of the particles depends on both coagulation and condensation onto the particles. The treatment of coagulation in the model is based on Brownian motion,

which is the major factor responsible for coagulation of submicrometre particles, and is recalculated as a function of particle size at each time step.

Particle growth also includes condensation of low volatile organics onto the particle following Nano-Köhler theory and adsorption of ammonia and water at each time step based on the equilibrium between the particle sulphate and water soluble organic content and the corrected ZSR approach based on hydroscopicity measurements made in Finland respectively.

Dry deposition of the particles is performed by applying the size dependant treatment of deposition velocities from Rannik et al. (2003)(Rannik, Aalto et al. 2003).

The performance of the UHMA model has been validated in a number of studies(Pirjola, Kulmala et al. 1999; Korhonen, Lehtinen et al. 2003). In addition, Korhonen et al. (2004)(Korhonen, Lehtinen et al. 2004) investigated the model with respect to a new particle formation event similar to particle formation events observed over a forest(Makela, Koponen et al. 2000). They show that the model predicts well the total particle number with the retracking the moving centre method best describing temporal growth. However, the model over predicted the total number concentration in the morning and failed to predict a sharp increase in particle number concentration in the afternoon; the failure in the latter case was explained as a result of the air mass properties at the measurement site.

In a second study Korhonen et al. (2003)(Korhonen, Lehtinen et al. 2003) examined the ability of two modelling approaches commonly used to represent particle size distribution within atmospheric modelling, to simulate new particle formation and growth.

They found that the fixed sectional approach was better able to predict the total particle concentration than the monodisperse approach, as used in MONO32, since the

monodisperse approach was unable to model the coagulation of newly formed particles. The authors observed that when the number of size sections in the fixed sectional approach is reduced the ability to accurately resolve changes in the particle size distribution decreased. However, the greater computational power required for the higher size resolution approaches within the sectional method means such an approach cannot be used in large scale dispersion studies. The simpler monodisperse method can be applied to larger scale studies as the authors demonstrated that it adequately estimated total particle number concentration and median particle size of the different modes

4. Overview of Urban and Regional Scale dispersion models

There are several regional dispersion models that calculate PM_{10} and $PM_{2.5}$ concentrations without calculating the particle size distribution. Many of these are used for regulatory purposes such as CALPUFF and TAPM(Hurley, Manins et al. 2003). Several larger scale models exist designed to model the aerosol dynamics within an urban airshed and regional scale, including the Urban Airshed Model with Aerosols (AERO-UAM IV), MADRID(Zhang, Pun et al. 2004), AEROFOR2(Pirjola and Kulmala 2001), Air Quality Model with Aerosols (Pai et al. 2000)(Pai, Vijayaraghavan et al. 2000), the California/Carnegie-Mellon Institute of Technology models of Meng et al. (1998)(Meng, Dabdub et al. 1998) and Pilinis and Seinfeld (1988)(Pilinis and Seinfeld 1988) and the Regional Particulate Model(Binkowski and Shankar 1995) (include other models). These models use a separate module to describe the aerosol dynamics coupled to a host air quality model, which is used to model the particle dispersion.

The treatment of aerosol dynamics is separate from the dispersion modelling and if the dynamics module can be integrated into a new dispersion model it is possible to incorporate the same aerosol dynamics approach using different dispersion strategies. This means that the comparison of air quality validation studies is difficult as the particle concentration is not only affected by the treatment of the aerosol dynamics but also a function of the particle dispersion.

4.1. Models that exclude specific treatment of aerosol dynamics

4.1.1. Box Models

The Photochemical Box Model (PBM, US EPA) is an extension of simpler box models that simulates photochemical smog at an urban scale. Similar to other box models it has a fixed area, typical horizontal dimensions are on the order of 10-50 km, but unlike other box models it has a variable boundary height between 0.1 and 2 km, consistent with the observed diurnal variation. It is suited to deal with low and variable wind conditions in the presence of sunlight. The urban area is represented by one or a set of cells within which the hourly concentrations of hydrocarbons and ozone are calculated. The PBM assumes that emissions, from point, line or area sources, are homogeneously distributed across the surface of the box and that the volume within the box is well mixed. After inputting the initial pollutant concentrations, hourly wind speeds, emission fluxes of CO, NO_x and HCs the model uses an extensive chemical reaction scheme and photolysis rates in junction with solar irradiance to simulate the formation of pollutants within the box.

4.1.2. Gaussian Models

AEROPOL is a steady state dispersion model for inert gases and particles upto 100 km from the source. It can also be used for local scale dispersion. It is only applicable to flat terrain, although treatment of building effects are included. The model includes an algorithm for plume rise based on the equations developed by Briggs (1975)(Briggs 1975). The model calculates wet deposition as a function of precipitation amount and dry using the deposition velocity approach. Atmospheric stability is calculated as functions of the Pasquill stability and the authors recommend it is used for dispersion in nearly neutral conditions and long term averages. In a comparison with the results from the Copenhagen data set, which corresponded to an elevated release within an urban environment in a neutral or slightly unstable atmosphere(Kaasik and Kimmel 2003) the modelled concentrations correlated well with the measured concentrations (R^2=0.64). However, the results correlated worse with the data set than the ADMS-UK but had a smaller tendency to calculate extreme deviations, as represented by the fraction of the values within a factor of 2 of the measured value (FA2) and NMSE values. The ADMS-UK comparison was performed at a much earlier state of development than its current state and so the ADMS-UK is currently at a more advanced development stage than AEROPOL. AEROPOL was not specifically applied to the dispersion of particles but the authors claim that the model is applicable to the dispersion of particles from stacks, vehicles and area sources.

CALPUFF is a multi-layer non steady state puff dispersion model designed to model the dispersion of gases and particles using space and time varying meteorology based on similarity equations, turbulence, emission strengths, transformation and removal. It is able to model four different source types: point, line, volume and area using an integrated puff formulation incorporating the effects of plume rise, partial penetration,

buoyant and momentum plume rise, stack effects and building effects using either the Schulman-Scire(Schulman, Strimaitis et al. 2000) or Huber-Snyder methods. The model calculates dry deposition using the resistance method with inputs for deposition velocities and wet removal using a scavenging coefficient approach as a function of precipitation intensity and type. Chemical transformations within the plume are based on the MESOPUFF method, which is a pseudo first order chemical mechanism for SO_2, and is able to include user defined diurnal cycles of transformation rates. As a result CALPUFF is not recommended for use in estimating the impact of NO_x and SO_2 on secondary PM formation less than 10km from the source. The model does not include any modelling of the particle dynamics. It provides hourly calculations of gas and particle concentrations from multiple emission sources in terms of particle mass but does not examine particle number concentration or size distribution.

CALPUFF has been used in a number of studies to investigate gas dispersion(US EPA 1998; Elbir 2003) and has been recently used to simulate a particle pollution episode that occurred during the winter over Christchurch(Barna and Gimson 2002). Validation studies showed good correlation with the two gas studies. Also the predicted hourly PM_{10} concentrations agreed well (Index of agreement, IA ranged from 0.67 to 0.87) with measured concentrations during a week in winter over Christchurch. In a study of the dust blown from erosion sources within the Mexico City basin(Villasenor, Lopez-Villegas et al. 2003) various levels of agreement were observed between the modelled and measured data. Villasenor et al. (2003)(Villasenor, Lopez-Villegas et al. 2003) concluded that the days with poorer correlations were a result of a different source. In a second study(Villasenor, Magdaleno et al. 2003), CALPUFF failed to predict the SO_2 concentrations in a complex environment among several gas and oil exploration and production sites in

south east Mexico. The model underpredicted the SO_2 concentrations and also showed poor temporal agreement. In general, CALPUFF showed reasonable agreement with pollutant concentrations in the validation studies and discrepancies appeared to the result of unknown sources. However, due to the inherent limitation CALPUFF is not recommended for calculation of timescales shorter than 1 hour or where dispersion is heavily influenced by turbulence such as in an urban environment.

AERMOD (AMS/US EPA) is a near field steady state Gaussian plume model based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources over both simple and complex terrain. It is able to model multiple sources of different types including point, area and volume sources. In the stable boundary layer the distribution is assumed to be Gaussian in both the horizontal and vertical directions. However, in the convective boundary layer (CBL) the vertical distribution is described using a bi-Gaussian probability density function, developed by Willis and Deardorff (1981)(Willis and Deardorff 1981), whilst the horizontal distribution is again considered to be Gaussian in nature. AERMOD is able to model buoyant plumes and incorporates a treatment of lofting, whereby the plume remains near the top of the boundary layer before mixing with the CBL. In general, Gaussian models are limited to treatment of flows over a simple terrain however, AERMOD incorporates a simple method to approximate flows over complex terrain (Snyder et al. 1985)(Snyder, Thompson et al. 1985).

The atmosphere is described by similarity scaling relationships using only a single measurement of surface wind speed, direction and temperature to predict vertical profiles of wind speed and direction, temperature, turbulence and temperature

gradient. The model does not include dry or wet deposition of gases and only includes a simple treatment of dry deposition using a reflection algorithm.

Whilst AERMOD is designed to model particle dispersion it has currently only been used to investigate gas phase dispersion. One gas phase study investigated it ability to model dispersion of an inert tracer in an urban environment. Venkatram simulated the emission from a small source on top of a building in an urban area SF_6 was released from a line source from the top of a trailer in a car park(Venkatram 2003). He observed that AERMOD over predicted average 30 minute concentrations at the upper end and underpredicted concentrations at the lower end of the measured concentrations at 24 receptor locations. However, AERMOD agrees within a factor of two of most of the middle concentrations. The agreement between modelled and measured concentrations at the closest receptors both in front of and behind the source was poor, especially at nighttime. The correlation improved with distance and showed better agreement with most of the data within a factor of two of the measured concentrations.

UK-ADMS is a UK regulatory model developed to model the dispersion of buoyant or neutrally buoyant particles and gases(Carruthers, Holroy et al. 1994). The model predicts the boundary layer structure using the similarity scaling approach in a similar method to Berkowicz et al. (1986)(Berkowicz, Olesen et al. 1986). The model uses an advanced Gaussian approach with a normal Gaussian distribution in stable and neutral conditions whilst the vertical dispersion is approximated by two different Gaussian distributions in a CBL. The treatment of the reflection of the plume of the surface of the earth is similar to other Gaussian models. ADMS calculates the plume rise based on temperature differences between the atmosphere and the emitted plume and

horizontal and vertical momentum fluxes including the possibility for entrainment of the plume and escape through the inversion at the top of the boundary layer.

The dry deposition of particles is modelled as a function of gravitational settling and deposition velocity with respect to aerodynamic, sub-layer and surface resistances. Wet deposition is approximated using a washout coefficient derived from the precipitation rate.

ADMS-Urban (and some other advanced Gaussian plume models) include buildings downwash algorithms and can model the effect of buildings, near wake recirculation and changes in the plume centre line due to streamline deflections from the buildings. However, the description of the canyon is limited and alignment of the canyons restricted limiting its application to urban particle modelling. The changing wind flow over complex terrain is calculated using FLOWSTAR, an advanced airflow model developed by CERC. Carruthers et al. (1988)(Carruthers, Hunt et al. 1988) have shown that FLOWSTAR models the flow well between tens of metres upto several kilometres typically for gradients between 1 in 2 (upwind slopes and hill summits) and 1 in 3 locally in hill wakes.

Hanna et al. (2001)(Hanna, Egan et al. 2001) compared the results of ADMS and AERMOD to five sets of field measurements, which represent a cross-section of scenarios common in modelling studies. In general both models performed well for all scenarios; however, there were some significant discrepancies. Following a ground level emission both ADMS and AERMOD underpredicted the concentration by a factor of three close to the source due to downwash effects of nearby tanks. Overall, both ADMS and AERMOD tended to underpredict the mean and maximum concentrations.

Carruthers et al. (2000)(Carruthers, Edmunds et al. 2000) compared the results of ADMS to measurements from urban and industrial locations in London, Ireland and Wales. In the urban environment they modelled the emissions within a 1 km grid from major point sources and roads with more than 25000 vehicles per day. ADMS predicted NO_x concentrations agreed well with the measured values but tended to underpredict at nighttime and in winter. Predicted SO_2 concentrations correlated poorer and were observed to be very sensitive to wind direction. In the industrial case again NO_x concentrations correlated well with the measured values except during low wind speed conditions. However, the PM_{10} and benzene concentrations were both significantly underpredicted. The authors suggest that this could be due to emission sources or strengths being poorly defined and the exclusion of periodic releases from the modelling. In addition, the agreement of the predictions with the modelled data improved when the complex terrain surrounding the site was included in the model description. In Belfast the model again significantly underpredicted the PM_{10} concentrations. Although the authors did not identify the cause of the discrepancy but suggested that they may result from regional variations in the background concentrations or the use of incorrect emission factors as they observed that domestic and traffic sources contributed significantly to the PM_{10} concentrations.

A recent comparison(Riddle, Carruthers et al. 2004) between FLUENT (a CFD model) and ADMS to predict dispersion from an isolated stack in neutral conditions over flat terrain showed that the Lagrangian particle approach within FLUENT gave similar results to ADMS but required much greater processing time. However, the authors stressed that the CFD models were more appropriate for situations in complex environments than ADMS.

SCREEN3(USEPA 1995) is a single source Gaussian plume model that is used for regulatory purposes to calculate the concentrations upto 50km from industrial emissions for worst-case scenarios. It is capable of modelling the dispersion of point, area and volume sources, the latter two through a numerical integration and virtual point source approach respectively. The atmospheric stability is calculated from Turner stability classes (similar to the Pasquill classification) and uses 10 m wind speeds to calculate the horizontal wind speed by correcting wind speeds at heights above 10m using a power law. The model incorporates an algorithm to calculate the building downwash effects for both far wake and near wake regions based on the Schulman-Scire(Schulman and Scire 1993) and Huber-Snyder schemes. The model uses results from Hosker (1984)(Hosker 1984) to calculate recirculation within a cavity. The calculated concentration is a function of building area, wind speed and source strength, and therefore sensitive to building orientation.

The effect of inversion break up is based on procedures in the Workbook of Atmospheric Dispersion Estimates (Turner 1970) and includes considerations due to plume rise but ignores the effects of elevated terrain. The calculation assumes a stable wind category and a fixed wind speed of 2.5 m s^{-1}. A similar treatment is applied to the shoreline fumigation and the maximum ground level shoreline fumigation is assumed to occur where the top of the stable plume intersects with the top of the well mixed thermal boundary layer. Buoyancy plume effects are based on the treatment of plume rise developed by Briggs (1975)(Briggs 1975) and used to adjust the vertical and horizontal dispersion coefficients.

SCREEN3 can calculate the effect of simple elevated terrain and also the 24 hour concentration due to plume impaction in complex terrain using the VALLEY module in which the receptors are located above the stack release height(Burt 1977) assuming

a stable atmosphere and fixed wind speed. It is claimed that the model can calculate the concentrations in flat or elevated simple terrain upto 100km, although the inherent limitations of the Gaussian plume equation mean that any estimations must be treated with extreme caution due to changes in wind field strengths and chemistry within the plume over this distance. No validation studies exist for SCREEN3; however validation studies of SCREEN(Mehdizadeh and Rifai 2004) and SCREEN2(Patel and Kumar 1998) show poor agreement with average measurements as they are designed to predict maximum hourly concentrations for worst case scenarios, in which the winds are not equally distributed from all directions. SCREEN3 is an updated version of SCREEN; however, the only algorithm that has been added that will affect the dispersion calculation is an alternative building downwash algorithm(Schulman and Scire 1993), which is unlikely to significantly affect the predictions of the validation studies discussed above.

4.1.3. Eulerian and Lagrangian Models

TAPM is an Eulerian grid based regional dispersion model that includes a Lagrangian particle mode for near source concentrations.

The atmosphere is treated as an incompressible non-hydrostatic fluid with the horizontal wind components determined from the momentum equations. It includes treatment of cloud processes and boundary layer parameterisation using similarity scaling and a k-ε solution to turbulence. Surface boundary conditions include changes to surface temperature and moisture for different soil and land use types based on the treatment by Kowalcysk et al. (1991)(Kowalcysk, Garratt et al. 1991).

Dry deposition is treated using a resistance method described by Physick and Garratt (1995)(Physick and Garratt 1995) in which the scalars behave like heat in terms of roughness and stability function with surface resistance based on surface type.

Wet deposition is only included for highly soluble gases and particles with the partitioning calculated as a ratio of the liquid-rain water volume fraction.

Gas-phase photochemistry is based on the generic reaction set (GRS), the semi-empirical mechanism developed by Azzi et al. (1992)(Azzi, Johnson et al. 1992) including the hydrogen peroxide modification(Venkatram, Karamchandani et al. 1997) and gas and aqueous phase reactions of SO_2 and particles based on Seinfeld and Pandis (1998)(Seinfeld and Pandis 1998). However, no aerosol dynamic module is included to describe changes to particle size distribution or particle number concentration. Comparison of the modelled particle mass concentrations with measured data showed good agreement for average and maximum particle concentrations in a year long study in Melbourne(Hurley, Manins et al. 2003).

TAPM was evaluated against two of the model validation kit studies from Indianapolis and Kincaid(Luhar and Hurley 2003), which simulated typical rural and urban concentrations in flat terrain. When compared with CALPUFF and AERMOD, TAPM performed as well and the agreement was even better when the observed winds were assimilated. The authors concluded that this showed that TAPM provides an accurate prediction of the local meteorology. From the results it was observed that TAPM tended to predict too low concentrations in nighttime, stable or neutral conditions and slightly too high concentrations during daytime convective or neutral conditions. Also locations of the maxima were slightly wrong during low wind events due to difficulties predicting the meandering of the flow.

A year long study(Hurley, Manins et al. 2003) of hourly averaged concentrations of O_3, NO_2, PM_{10} and $PM_{2.5}$ was performed comparing the predictions with concentrations measured across Melbourne using a detailed emission inventory for vehicle, commercial, domestic and biogenic sources.

They observed that TAPM tended to underpredict daily PM_{10} and $PM_{2.5}$ concentrations averaged across all sites by about 13%. No correlation between hourly concentrations was made due to the fact that particle air quality standards were based on 24hr averages.

Despite slightly underpredicting annual NO_2 average the model showed excellent agreement with the maximum NO_2 concentrations and very good agreement with the O_3 and particle concentrations. The underprediction of the NO_2 was due to differences in the winter and nighttime concentrations. The results also showed that TAPM accurately predicted concentrations even when no meteorological data was taken.

In a further study (Hurley, Blockley et al. 2001), TAPM predicted hourly wind and temperature values agreed with observed values at each site (IA = 0.84 and 0.96 respectively). SO_2 concentrations showed good correlation with the measured concentrations and a modelled annual average of 94 $\mu g\ m^{-3}$ compared excellently with the observed average over all sites of 95 $\mu g\ m^{-3}$.

ARIA Regional model has been developed in order to analyse the dispersion of gases and particles, coming from industrial, transportation and area sources, upto 1000km with a resolution of between 1 km and 10 km. ARIA can process multi- and single constituent isothermal and non isothermal gas flows as a function of the thermodynamic properties of the gases.

The meteorological model incorporates a turbulence and deposition processor and is able to calculate wind flows over simple and complex terrain from microscale to synoptic scale that are based on the solution of the atmospheric motion equation and a closure model for the Reynolds stresses(Pielke, Cotton et al. 1992). The mean wind velocity is calculated using a mass consistent model to generate 3-D wind and temperature profiles. The treatment of turbulence uses the parameterisation approach of Hanna 1982(Hanna 1982) based on similarity scaling.

ARIA Regional model uses two different theoretical approaches allowing the user to choose the most suitable dispersion model for the application: FARM model, which is based on Eulerian approach and SPRAY which is based on Lagrangian approach. FARM is used to calculate concentration and deposition of reactive emissions including photochemistry gases and particles between 50 and 1000 km, while SPRAY is proposed to determine concentration and deposition of non-reactive emissions over complex terrain and focuses on particle emissions. The model calculates dispersion using either a one or two way nesting within multiple grids.

The model incorporates treatment of the thermodynamic equilibrium between the gas and condensed phases and includes treatment of wet and dry deposition and radioactive decay.

SPRAY model is a Lagrangian particle model capable of calculating dispersion for multiple sources within micro to regional scales based on the generalised Langevin equation for inhomogeneous and non Gaussian turbulence(Thomson 1987). The model has been developed and used to study the dispersion of passive pollutants in complex terrain(Nanni, Riva et al. 1996; Anfossi, Desiato et al. 1998; Carvalho, Degrazia et al. 2002; Gariazzo, Pelliccioni et al. 2004). SPRAY has been

updated(Ferrero, Anfossi et al. 2000) to include the Gram-Charlier probability density function to solve the Fokker-Plank equation.

A recent study of SPRAY(Gariazzo, Pelliccioni et al. 2004) showed that despite accurately calculating the wind speeds, although some discrepancies were observed in the frictional velocity, agreement was in general very good. This was thought to be result of problems of the model to take vertical remixing of the atmosphere into account. Another problem of the model was the calculation of daytime turbulence, which is strongly affect by thermal convection. Therefore, some differences existed in the agreement although the model was able to reproduce the general behaviour of the diurnal turbulence cycle. During the study period the model in general showed reasonable agreement with measured NO_x and SO_2 concentration with a few major exceptions. These occurred during periods corresponding to upwind conditions when the modelled emissions were not expected to impact on the measurement locations.

4.2. Regional Aerosol models involving detailed treatment of Aerosol dynamics

The CIT model, designed to model dispersion within an urban airshed, incorporates the aerosol model of Pilinis and Seinfeld (1988)(Pilinis and Seinfeld 1988). The model uses a sectional approach to particle size distribution with three size sections between 0.05 and 10 μm and the aerosols composed of a mixture of organic and inorganic compounds. Nucleation was assumed to occur using only classical theory of binary nucleation involving sulphuric acid and water. In order to reduce the computational requirement of mass transfer of volatile species and due to uncertainties in ambient aerosol measurement the model assumes that the aerosols are in thermodynamic equilibrium. They use an inorganic equilibrium model that predicts gas phases concentration of NH_3, HCl and HNO_3 and aerosol phase concentrations of

H_2O, NH_4^+, SO_4^{2-}, NO_3^-, Na^+, Cl^-, HSO_4^-, H_2SO_4, Na_2SO_4, $NaHSO_4$, NaCl, $NaNO_3$, NH_4Cl, NH_4NO_3, $(NH_4)_2SO_4$, NH_4HSO_4 and $(NH_4)_3H\ (SO_4)_2$. Gas phase chemistry was modelled using the mechanisms of Russell et al. (1988)(Russell 1988). Secondary aerosol formation is assumed to be from three sources: aromatics, diolefins and the cyclic ethenes, cyclopentene and cyclohexene. The dispersion model assumes that the atmosphere exists of 5 unequally distributed layers upto 1100m with a horizontal size of 150 km x 400km divided into 5x5 km grid squares.

The URM-1ATM model is an updated version of the CIT model and calculates the dispersion and chemistry of the pollutants by solving the Eulerian equations for conservation of mass using a finite element variable transport scheme coupled to the updated SAPRC chemical mechanism(Carter 2000; Carter 2003). Aerosol dynamics are modelled using a sectional approach with four size groups upto 10μm made up of internally mixed atmospherically relevant particles. The equilibrium based model ISORROPIA(Nenes, Pandis et al. 1998; Nenes, Pandis et al. 1999) is used to calculate the growth and mass transfer of particles through condensation. The module ISORROPIA designed to calculate the gas-aerosol partitioning of inorganic compounds is very computationally demanding. Recently Metzger et al. (2002)(Metzger, Dentener et al. 2002) have developed a simpler model, EQSAM, that assumes chemical equilibrium to relate the aerosol activity coefficients to relative humidity. Metzger et al. (2002)(Metzger, Dentener et al. 2002) showed that EQSAM was much faster and provided comparable results to ISORROPIA using a non iterative manner. They concluded that it provides a good alternative to ISORROPIA in global modelling applications.

The model incorporates a wet deposition and scavenging process developed by Berkowitz et al. (1989)(Berkowicz, Easter et al. 1989) to simulate the formation of clouds and kinetic interaction with the atmospheric species. The dry deposition of the particles uses the three resistance approach as described by Wesely (1989)(Wesely 1989).

Lurmann et al. (1997)(Lurmann, Wexler et al. 1997) coupled the AERO model dispersion model to UAM IV, which is a similar aerosol model to that employed by Pilinis and Seinfeld (1988)(Pilinis and Seinfeld 1988). Size distribution was represented by eight sections between 0.04 and 10 μm and assumed uniform composition of aerosols composed of inorganic and organic compounds and elemental carbon. Nucleation and condensation were identical to the treatment by Pilinis and Seinfeld (1988)(Pilinis and Seinfeld 1988). Only dry deposition was considered using the method recommended by Slinn and Slinn (1980)(Slinn and Slinn 1980) to calculate the deposition velocities. The effects of changing season and land cover on surface resistance were calculated using the approach of Wesely (1989)(Wesely 1989).

The model was used to reproduce concentrations measured during two summer pollution episodes in Los Angeles in 1987. The AERO-UAM IV performed poorly with respect to the observed NO_2 concentrations generally tending to underpredict the hourly concentrations. Modelled ozone concentrations showed the desired trends but often over and underpredicted the observed concentrations with a mean error of ± 35%. The model predictions for mean daily $PM_{2.5}$ mass agrees relatively well with the observed mass. Elemental carbon and crustal material was found to make up the major component of aerosols greater than 1.2 μm with nitrate ions accounting for

about 50% of the mass of aerosols smaller than 310nm. The authors commented that the good agreement between the measured and modelled $PM_{2.5}$ was a result of the overestimation of the crustal emissions since several of the individual contributions were underestimated. Predictions of the 24 hr and 4hr PM_{10} mass concentrations were higher than observed at all locations. Further examination of the individual components of the PM_{10} particles showed that the model again over estimated the crustal component but underpredicted a number of the other components of the aerosols. The most accurate component of PM_{10} was nitrate which is surprising due the underprediction of the NO_2 and nitric acid, which influence the formation of nitrate ion.

CALGRID is a Eulerian dispersion model based on the UAM-IV model with improvements to the horizontal advection(Yamartino, Scire et al. 1989), vertical transport, deposition and chemical transformation(Scire and Yamartino 1989).

CALGRID uses regularly spaced horizontal grid sizes between 500 m and 20km and vertical height from 20m to 2km to create a horizontal domain between 20-1000 km and height upto 10km to calculate hourly concentrations of both reactive and inert gases and particles within a complex terrain. Atmospheric stability and boundary layer height is calculated using stability categories (Briggs 1973). Vertical diffusivity is based on convective scaling during the day and local scaling at night. Plume rise of buoyant sources within a stable, neutral or unstable atmosphere is calculated using the treatment of Briggs (1975)(Briggs 1975).

Emissions are generated for each cell and each species in terms of mass per unit time.

CALGRID includes the photochemical mechanism SAPRC to predict the formation of secondary gases. The treatment of aerosols includes both primary particles and

SOA formation. Particles are formed using the Chemical Bond Mechanism IV (CBM IV) containing 86 reactions and 35 species (Gery, Whitten et al. 1989). In addition, the chemical thermodynamic model ISORROPIA to provide detailed treatment of equilibrium and partitioning between gas, liquid and solid phases.

SOA formation is a function of reaction rate and stoichiometry of the reactions as well as a temperature dependent equilibrium partitioning dynamics. Ultraviolet (uv) irradiance in each cell is a function of cloud cover and includes an algorithm for transmissivity developed by Bais et al. (1993)(Bais, Zerefos et al. 1993) and the effects of surface albedo to provide the total uv flux in a layer. This flux is used to calculate the photolysis rates.

Three options are available for dry deposition depending on the complexity of the calculation. The user can choose to ignore dry deposition, define 24 hour cycles of the deposition velocities or calculate deposition rates as a function of space and time, based on the equations of Wesley and Hicks (1977)(Wesely and Hicks 1977) for gases and as a function of particle size using the equations from Slinn and Slinn (1980) (Slinn and Slinn 1980) and Pleim et al (1984)(Pleim, Venkatram et al. 1984). No treatment is included for wet deposition.

O'Niell and Lamb (2005)(O'Neill and Lamb 2005) compared the results for CALGRID coupled to the photochemical model SAPCR97 with measured O_3 concentrations. They showed that the hourly model results correlated very well with the measured concentrations. This study demonstrated that the formation of one of the major secondary pollutants, critical to the accurate determination of particle formation is accurately modelled by the photochemical mechanism included in CALGRID.

Villasenor et al. (2001) (Villasenor, Claiborn et al. 2001) modelled PM_{10} and $PM_{2.5}$ concentrations using CALGRID in industrial and residential areas. They did not

include the photochemical mechanism, SAPRC. The model correlated excellently (R^2=0.94) with the measured hourly PM_{10} values and slightly less well but still showed a good correlation with $PM_{2.5}$ values (R^2=0.63). The reduced correlation of the $PM_{2.5}$ values was probably a reflection of the small influence that traffic emissions have at the sites. However, the absence of chemical transformations would also have more affect on the $PM_{2.5}$ correlation than the PM_{10} since the percentage contribution of particle formation to the $PM_{2.5}$ should be greater.

UNI-AERO is an aerosol model that incorporates the EMEP dispersion model within equidistance 50 x 50km horizontal grid cells and 20 size varying vertical layers. Horizontal and vertical advection are determined according to schemes designed by Bott(Bott 1989). Atmospheric Stability is calculated using similarity theory and vertical diffusivity calculated from local Richardson numbers as a function of the atmospheric stability.

The model includes treatment of both primary and secondary particles, although SOAs are not currently included in the standard version. Chemistry includes a full photochemical mechanism(Kuhn, Builtjes et al. 1998) together with ammonium chemistry, gas and aqueous oxidation of SO to sulphate. Partitioning of semi volatile inorganic compounds between the gas and aerosol phases is calculated using ESQAM, which also calculates water associated with the aerosols based on chemical composition using the ZSR relationship(Robinson and Stokes 1965). In this way the aerosol water content calculated depends on the mass of soluble compounds and type of salt mixture in the particle.

UNI-AERO calculates particle mass and number concentration in four modes as a function of aerosol chemical composition, thus allowing the user more choice in the

cut off of aerosol diameter in PM_x. Aerosol dynamics includes treatment of binary and ternary nucleation(Korhonen, Kulmala et al. 1999; Berndt, Boege et al. 2000), condensation and coagulation in addition to deposition.

Dry deposition is calculated using the resistance method as described by Wesley et al (1989) (Wesely 1989)with the velocity in each cell moderated as a function of fractional land use within each cell. Wet deposition of soluble components is treated using both in-cloud and sub cloud equations, which are functions of the precipitation rates and in-cloud and sub-cloud scavenging ratios

Tsyro et al. (2003)(Tsyro 2003) has observed that UNI-AERO (described as EMEP Aerosol model) systematically underestimated the observed $PM_{2.5}$ and PM_{10} concentrations by between 40 and 60 percent. They concluded that the discrepancy could result from SOA that are not included in the model. They investigated the influence of different factors on the model calculations. Inclusion of the photochemistry model in contrast to the simplified treatment had the largest effect whilst the effects of deposition and aerosol dynamics had only a minimal difference between the model performance. This confirmed that the regional modelling of PM_{10} can be adequately performed without inclusion of aerosol dynamics.

A second study, Tsyro et al. (2005) (Tsyro 2005), investigated whether the difference between the modelled and observed $PM_{2.5}$ and PM_{10} concentrations could be a result of the water content of the aerosols. They found that the unaccounted for $PM_{2.5}$ mass at two sites correlated well with the calculated residual aerosol water. When the water associated with the aerosol was include in the model predictions the authors observed that at most sites the daily the agreement of PM_{10} and $PM_{2.5}$ concentrations with the measured values improved, though there were some notable exceptions where the correlation worsened. They postulated that this was because of the atmospheric

conditions used by the model, in particular temperature and humidity. Despite the improved agreement they showed that significant fractions of the $PM_{2.5}$ and PM_{10} mass were unidentified. They showed that the chemical composition of the PM_{10} aerosol calculated by the model correlates very well (R^2 was between 0.55 and 0.69) with the measured aerosol composition.

Furthermore, the model showed good correlation with the daily $PM_{2.5}$ and PM_{10}, except for at the Spanish sites where the large discrepancy was due to the absence of wind blown dust in the model.

The regional particulate matter (RPM) model includes a treatment of particle dynamics incorporated into the RADM II dispersion model(Binkowski and Roselle 2003). The model approximates the size distribution using two discrete particle sizes, representing nuclei and accumulation modes, approximated by a lognormal distribution centred about 0.01 and 0.07 μm respectively, composed of hydrates of ammonium sulphate and ammonium nitrate. Nucleation is again based on the homogeneous binary nucleation of sulphuric acid and water and includes a similar treatment of condensation, coagulation and deposition used by Pilinis and Seinfeld (1988)(Pilinis and Seinfeld 1988). The thermodynamic equilibrium within the aerosol phase is calculated using the model developed by Saxena et al. (1986)(Saxena, Hudischewskyi et al. 1986).

Gas phase chemistry within the model is described by the second generation chemical mechanism developed by Stockwell et al. (1990)(Stockwell, Middleton et al. 1990) which has since been updated to the RACM mechanism. This includes updated rate constants and product yields from laboratory measurements and includes the new condensed reaction mechanism for isoprene, α-pinene, and δ-limonene with different

branching ratios for alkane decay. Additional changes were made to aldehyde and aromatic chemistry in line with more recent kinetic studies.

More recently Meng et al. (1998)(Meng, Dabdub et al. 1998) developed a three dimensional size resolved and chemically resolved aerosol model using the CIT dispersion model. The aerosol distribution function is based on a sectional approach, which allows individual description of the chemical composition of the aerosols within each size section. The model calculates the mass of the particles based on the sum of its individual components from the equations of Pilinis (1990)(Pilinis 1990). Based on the approach of Wexler et al. (1994)(Wexler, Lurmann et al. 1994) the model ignores the effect of coagulation on the aerosol growth but incorporates the binary nucleation of sulphuric acid, contrary to the treatment of condensation in the models of Pilinis and Seinfeld (1988)(Pilinis and Seinfeld 1988) and Lurmann *et al*. (1997)(Lurmann, Wexler et al. 1997) which assumed instantaneous gas-aerosol equilibrium. Condensation is modelled dynamically using the equation proposed by Wexler et al. (1994)(Wexler, Lurmann et al. 1994) and the dry deposition calculated from the equation of deposition velocity from Russell *et al*. (1993)(Russell, Winner et al. 1993).

In addition to the aerosol thermodynamics of the earlier models Meng et al. (1998)(Meng, Dabdub et al. 1998) incorporated the option of calculating the inorganic gas-aerosol equilibrium by Kusik-Meissner(Kusik and Meissner 1978) and Pitzer methods(Pitzer and Kim 1974) with respect to variations in both temperature and relative humidity. As with the other models the water activity is estimated by the ZSR method(Robinson and Stokes 1965) because it is as accurate as more complex methods and requires significantly less computer power.

AEROFOR2(Pirjola and Kulmala 2001) uses a sectional modelling approach of over 200 evenly distributed size sections with logarithmic distribution within each section. The composition of the aerosols within each section can be varied for soluble, weakly soluble and insoluble particles and through the temporal treatment of the dynamics it is possible to follow the particle number concentration as well as composition with time. The nucleation includes formation through both homogeneous binary nucleation and ternary nucleation, as discussed above. The model includes a multicomponent approach to condensation of H_2SO_4, H_2O and organic compounds on the existing aerosols. Condensation of sulphuric acid and organic compounds depends on the concentration difference between the gas and surface concentrations but the thermodynamics of the condensation of the organic compounds is not considered since the individual identity of the compound is not specified. Changes in solubility and size of the particles due to condensation are calculated and growth of the particles adjusted due to hygroscopic absorption of water.

Coagulation of the particles is based on Brownian coagulation coefficients(Fuchs 1964) and redistribution of the size classification is done simultaneously with condensation effects. Dry deposition of the particles assumes Brownian diffusion, interception and gravitational settling rates according to Schack et al. 1985(Schack Jr, Pratsinis et al. 1985).

The gas phase chemistry is based on the EMEP mechanism(Simpson 1992), which includes 140 chemical and photochemical reactions for 68 compounds and requires the initial concentration, emission rate and deposition velocity for each compound.

The MADRID model(Zhang, Pun et al. 2004) was coupled to the Community multiscale air quality model (CMAQ) dispersion model in order to simulate the dispersion within the Los Angeles Basin. MADRID uses a multiple size sectional approach with internally mixed particles to describe the size distribution. The model includes explicit treatment of all processes except for coagulation. A parameterized version based on the method of McMurray and Frielander (1979)(McMurray and Frielander 1979) is used to simulate new particle formation and condensation onto existing particles. The thermodynamics of the inorganic aerosol species is modelled using ISORROPIA. Two approaches to the formation of SOA have been used one based on the more comprehensive CACM mechanism and the other on the CBM-IV or RADM approaches with additional treatment of aromatics and biogenic volatile organic compounds. A mixing approach similar to that described by Jacobson is used to describe the condensation, with the Carnegie-Mellon University (CMU) approach(Capaldo, Pilinis et al. 2000) used to calculate mass transfer of gases to particles following a hybrid approach combining both equilibrium and dynamic(Capaldo, Pilinis et al. 2000; Pilinis, Capaldo et al. 2000) methods depending on the particle size. Dry deposition is described using the algorithm of Venkatram and Pleim (1999)(Venkatram and Pleim 1999) and wet deposition by the original CMAQ module(Binkowski and Roselle 2003) modified to include the effects of dissociation reaction by use of the effective Henry's Law constant. Also included in the model are cloud and aqueous phase processes previously used in the CMAQ model. These have been updated to include a comprehensive chemical mechanism to describe the aqueous phase chemistry and subroutines to estimate the activation of aerosols and scavenging by clouds including treatment of reformation of particles after cloud evaporation.

Heterogeneous reactions involving HO_2, NO_2, NO_3 and N_2O_5 on the surface of particles are included in the model either as part of the CMU bulk aqueous phase mechanism or individually.

5. Conclusion

This paper provides the first detailed review of dispersion modelling packages with reference to the dispersion of particles in the atmosphere. The models reviewed included: Box models (AURORA, CPB and PBM), Gaussian models (CALINE4, HIWAY2, CAR-FMI, OSPM, CALPUFF, AEROPOL, AERMOD, UK-ADMS, SCREEN3), Lagrangian/Eulerian Models (GRAL, TAPM, ARIA Regional), CFD models (ARIA Local, MISKAM, MICRO-CALGRID) and models which included aerosol dynamics (GATOR, MONO32, UHMA, CIT, AERO, RPM, AEROFOR2, CRM-1ATM, UNI-AERO, CALGRID, MADRID). It outlines differences between different model types and their limitations with respect to the scales and processes included. This review showed that considerable differences exist between the available model packages and due to the limitations of the models in terms of mathematical treatment of dispersion dynamics and treatment of the aerosol processes, considerable thought has to be given to the choice of the model for each application. Factors which are critical to the choice of the model include: the complexity of the environment, the dimensions of the model, the nature of the particle source, the computing power and time that is required and the accuracy and time scale of the calculated concentrations desired. Even with the most perfect model fluctuations in the wind flow and emission strengths mean that the results generated are only an approximation of the actual concentrations. Restrictions imposed due to the lack of time and computing power, in addition to the uncertainties in the

modelling parameters, such as emission factors and description of the atmosphere, mean that the relative importance of the individual factors must be assessed and the models used to provide concentrations within an appropriate degree of error and time period.

The applicability of the models to particle dispersion modelling depends heavily on the nature of the concentration desired. Whilst, the modelling of particle number concentration close to the source, for example in local and urban scales, requires in depth modelling of aerosol dynamics Tsyro et al. (2003)(Tsyro 2003) have shown that results for the UNI-AERO model indicate that aerosol dynamics has only a minor influence on particle mass concentrations in a larger regional scale. In addition, without the specific treatment of the chemistry and particle dynamics the dispersion models are best used to predict mass concentrations since they are typically based on the assumption of conservation of mass at each timestep. Therefore, within most approximations gas phase dispersion models seem reasonably accurate with respect to calculating average daily and annual particle mass concentrations in simple and regional domains.

Whilst not proposing to be a review of every model available this paper provides a source of information of applicability of the chosen model to the desired application. It is unfortunately not possible to rank the models in terms of best to worst table as comparison between the models and even a single validation data set has not been performed and studies have shown that whilst one model might perform better than an alternate model in one study the results may be reversed in a different scenario. Therefore, the order depends on modelling timescale required, domain environment and nature of the emission sources. Where possible comparison has been provided between the performance of two or more models with regards a particular validation

data set and the user is left to decide which data set is more appropriate to their study. We feel that major weaknesses in particle dispersion modelling exist a result of the lack of studies that simultaneously measure particle number concentration and gaseous pollutant concentrations and the lack of validation studies that compare the performances of the various models against validation data. The latter point is probably due to the fact that most of the aerosol dynamics models are not commercially available.

Name Developer	**Model Type**[1]	**Scale**[2]	**Grid Size**	**Resolution**	**Source Types**[3]	**Pollutants**[4]	**Output frequency**	**Atmospheric Stability**[5]	**Turbulence**[6]
AURORA VITO	B	L	1x1 km	NA	L	CO, NO_2, SO_2, PM_{10}	1 hr, 24 hr, 1 yr	NA	Limited AMB
CPB GEOMET	B	L		NA	L	NO_2 and inert gases		NA	NA
CALINE 4 Californian Department of Transportation	GP	L	H:100-500 m	1 m	L	CO, NO_2, TSP	1 hr, 8 hr, Worst case	P	VIT,AMB
HIWAY2 US EPA	GP	L	10-100 m but upto 10km depending on scaling factor	1 m	L	Non reactive gases	1 hr	P	VIT,AMB
CAR-FMI Finnish Met. Institute	GP	L	Upto 10 km	H: adjustable V: Not defined	L	CO, NO, NO_2, NO_x, $PM_{2.5}$	1 hr, 8hr, 24 hr, 1 yr	BL	VIT, AMB
AEROPOL Bulgaria	GP	L	H: Upto 100 km V: Upto 2 km	H: 10-1000m V: 100m	P,V	G,P	1 hr	P	AMB
ADMS CERC	3D quasi GP	L, R	3000 grid cells upto 50km	H: no limits V: no limits	P,A,L	G, P	10 mins to 1 yr	BL	VIT AMB
GRAL	L	L	100m-20km	H: no limits V: no limits	P,L	G, P	10 min to 1 hr	BL	Local (k-L model) Vertical inhomogeneous turbulence and inhomogeneous 3D wind fields
GATOR	E	L, R, G	Upto Global	Depends on scale of area	P,L,A,V	G, P	1 hr to 1 yr	BL	AMB
OSPM National Environmental Research Institute, Denmark	GP/Box	L	NA	NA	L	NO_x,NO_2, O_3, CO PM	1 hr	NA	VIT, Empirical wind turbulence
STAR-CD	CFD	L	<1 km	H:<1 m + V:<1m +	P,L,A,V	G, P	1 min	BL	VIT
ARIA Local ARIA Technologies	CFD	L	depends on scaling factor	H:<1 m + V:<1m +	P,L,A,V	G, P	Real time	P	VIT, Local (k-L model) Vertical inhomogeneous turbulence and inhomogeneous 3D wind fields
PBM	Box	R	H:<50 km V: variable <2 km	NA	P,L,A	G		NA	NA
CALPUFF Californian Department of Transportation	Multi layer non steady state GPuff	R	<200km	H: no limits V: no limits	P,L,A,V	G, P	> 1 hr	BL	AMB
SCREEN3	GP	R	<50km	H: no limits V: no limits	P,A,V	G, P	1hr in simple >24 in complex terrain	T Worst case scenario meteorology	Y
TAPM CSIRO, Australia	E/L	R	<1000 x 1000 km	H:0.3 -30 km V :> 10 m	P,A,V	G, P	1 hr, 8 hr, 1 yr	BL	k-ε
AERMOD American	Bi Gaussian	L, R	<50km	H: no limits	P,A,V, (L	G, P	1 hr, 24 hr, 1 yr	BL	AMB

Met. Society	Steady State GP			V: no limits	treated as series of V)				
SPRAY ARIA Technologies	L	L, R	<1-100 km	H: 1 m to 4 km V: 1 m to 4 km	P, L, V	G, P	1 min+	BL	
MISKAM	CFD	L	<300 m	H: 1m (60 cells in each direction) V: 1m (20 cells)	P, L, V	G, P	1 min+	BL	AMB
MICRO-CALGRID	CFD	L	<10 km	H: 1m V: 1m	P, L, V	G, P	1 min+	BL	VIT, AMB

NA = Not applicable
[1] Model Types: B = Box, G P = Gaussian Plume, L = Lagrangian, E = Eulerian, CFD = Computational Fluid Dynamics, GPuff = Gaussian Puff
[2] Scale: L = Local, R = Regional
[3] Source Types: L = Line, P = Point, A = Area, V = Volume
[4] Pollutants: G = Gases, P = Particles
[5] Atmospheric Stability: P = Pasquill, BL = Boundary Layer Scaling, T = Turner
[6] Tubulence: VIT = Vehicle Induced Turbulence, AMB = Turbulence of Ambient Air

Table 1a. Basic Parameters for Models not containing Aerosol Dynamics modules

Name Developer	**Street Canyon**	**Building Wake Effects**[1]	**Topography**	**Intersections**	**Plume Rise**	**Chemistry**	**Aerosol Dynamics**
AURORA VITO	Y	X	Simple	X	X	X	X
CPB GEOMET	Y	Y	Simple	X	X	X	X
CALINE 4 Californian Department of Transportation	X	X	Simple	Y	X	DPM	X
HIWAY2 US EPA	X	X	Simple	X	X	X	X
CAR-FMI Finnish Met. Institute	X	X	Simple	X	X	DPM	X
AEROPOL Bulgaria	X	X	Simple	X	Y	Y	Deposition
ADMS CERC	Y	Y	Complex	Y	Y	Y	X
GRAL		X	Complex	X	Y	X	X
GATOR	X	X	Simple	X	X	Y	Y
OSPM National Environmental Research Institute, Denmark	Y	Y	Simple	X		Y (NO-NO_2-O_3 chemistry)	X
STAR-CD	Y		Complex				
ARIA Local ARIA Technologies	Y	Y	Complex	Y	Y	Y	X
PBM	X	X	X	X	X	Y	
CALPUFF Californian Department of Transportation	X	S-S H-S	Complex	X	X	X	X
SCREEN3	Y	S-S H-S	Simple and Complex	X	X	X	X
TAPM CSIRO, Australia	X	S-S H-S	Complex	X	Y Simplified Glendinning et al. (1984)	Y GRS	X
AERMOD American Met. Society	X	Evaluation version	Simple and Complex	X	X	Y Simple SO_2 decay	X
SPRAY ARIA Technologies							
MISKAM	Y	Y	Simple	X	X	X Simple (NO-NO_2 conversion model)	X
MICRO-CALGRID	Y	Y	Simple and Complex	X	Y	Y	Y

X Not included, Y included

[1] Building Wake Effects: S-S = Schulman-Scire, H-S = Huber-Snyder

Table 1b. Processes included in the dispersion models not containing an Aerosol Dynamics package

Name Developer	Dispersion model	Nucleation[1]	Coagulation	Condensation / Evaporation	Deposition[2]	Particle Size method	Particle composition
UHMA University of Helsinki		B+T	Y	Y	D:Y W:X	Hybrid/ moving centre of retacking methods 0.7nm-2μm	H_2SO_4, Inorganics, Organics
MONO32	Coupled to OSPM	B+T	Y	Y	D: Y W: X	4 size modes. Monodisperse approach 7-450 nm	None
AERO	Coupled to UAM-IV	Y		Y	D: Y W: X	0.01-10μm	Inorganic, organic and elemental carbon. Internally mixed
GATOR	Eulerian	B	Y	Y	D: Y W: X	Moving size or stationary size	None
MADRID	Coupled to CAQM	SOA, B		Y	D: Y W: X	Multiple size sectional	
AEROFOR	Sectional Box	B,T	Y	Y	D: Y W: Y	200 groupings	Externally or internally mixed varying within each size group
URM	Eulerian	B	X	Y	D: Y W: Y	4 groups <10 μm	Internally mixed
RPM	Incorporated into RADMII	B	Y	Y	D: Y W: Y	0.01-0.07μm	Ammonium Sulphate Ammonium Nitrate
CIT Californian Institute of Technology		B	X	Y	D: Y W:X	0.5-10 μm	Organic Inorganics

Y = process included, X = process not included

[1] Nucleation: B = Binary, T = ternary, SOA = Secondary organic aerosol formation

[2] Deposition: D = Dry deposition, W = Wet deposition

Table 2. Aerosol Dynamics models

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