



Modelling Neighbourhood-Scale Dispersion of Ultrafine Particles

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Ultrafine nanoparticles (UFP; diameter < 100 nm) are respirable particles which cause health effects by accumulating in lungs and penetrating cells/tissue. The atmospheric transport and respirability of UFP are very size-dependent. Traffic is normally the most important source of UFP emissions in urban areas. Traffic-generated nanoparticles, vented out from an urban street network, can evaporate partially while they are transported during neighbourhood-scale dispersion. This study simulates the dispersion and evolution of nanoparticles, using as a case study the neighbourhood between Marylebone Road and Regent's Park in London, UK, for which new and previous measurements are available. A model for the microphysics of multicomponent UFP has been developed. The model is based on surrogate molecules (C16-C32 n-alkanes, which are the most abundant compounds in our laboratory two-dimensional gas chromatography studies of diesel emissions). We can then explore, in a structured and systematic way, the sensitivity of the UFP size distribution to changes in particle composition and saturation vapour pressure of the surrogates.

For mid-latitude ground-level conditions and over timescales (ca. 100 s) relevant for dispersion on the neighbourhood scale (i.e. up to 1 km), the choice of a particular vapour pressure dataset changes the range of compounds that are appreciably volatile by 2-6 carbon numbers. Model results, using a middle-of-the-range volatility expression, indicate that representation of the C22H46-C24H50 components is far more important than that of other surrogate components, which are either effectively volatile so as to equilibrate with the gas phase quickly or effectively involatile so as to vary negligibly in this setting. This offers a way to improve the computing efficiency of urban aerosol models by adopting simplified schemes for these less important components: e.g., an equilibrium scheme for low-carbon-number components and a linear scheme for high-carbon-number components.

The microphysics code has then been implemented in the WRF-LES modelling framework (Weather Research and Forecasting, WRF; Large Eddy Simulation, LES). Real-world gridded emissions are implemented in this 2.54 km x 2.54 km simulation representing a real-world street network, revealing the behavior of UFP dispersion. Nanoparticle composition is composed of 18 components: 1 non-volatile core and 17 surrogate n-alkane components. The number of sectional size bin is 15, ranging from about 6 nm to 500 nm in log-scale. 3D fields of particle mass for each surrogate component and for each size bin (a total of 15 [U+F0B4] 18=270 fields) and gas concentrations (a total of 18 fields) are tracked; i.e. the advection and diffusion of these quantities are solved by WRF-LES. The particle number for each size bin is diagnosed according to the mass concentration in each sectional size-bin. A gridded neighbourhood-scale street network in London with traffic-induced UFP emissions is incorporated into the model.