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ACCURATELY MODELLING UFP TRANSFORMATION PROCESSES INSIDE A TRAFFIC TUNNEL

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Abstract: There is increasing scientific evidence that the number concentration of (traffic related) ultrafine particles may be a better proxy for the adverse health effects due to particulate matter than the currently regulated PM_{10} and $PM_{2,5}$ mass fractions. However, no consensus has been reached whether UFP transformation processes (such as deposition, coagulation, condensation) should be taken into account for appropriately modelling the dispersion of UFP number concentrations within urban environments. Due to their confined space and the controlled conditions, traffic tunnels form the ideal environment to investigate this hypothesis.

We have developed a computational model that is able to predict the UFP size-distribution at every location within the tunnel. The model consists of a number of modules that implement the most important transport and transformation processes, i.e. emissions, advection, deposition, coagulation and condensation. The novelty of the model is that it is using state-of-the-art numerical methods that allow for a high-accurate and continuous representation of the solution.

We here present the results of a validation study that demonstrates that the model is able to accurately predict the evolution of the UFP size-distribution inside a traffic tunnel. Moreover, we present a novel approach to identify the dominant processes that govern the UFP size distribution by applying a size-resolved time-scale analysis.

Key words: *UFP, traffic tunnel, coagulation, condensation, deposition, time-scale analysis*

INTRODUCTION

Because of its adverse impact on human health, the air pollution due to particulate matter (PM) is an environmental problem of major concern. Although their number concentration may be high, ultrafine particles (UFP, particles less than 100 nm in diameter) barely contribute to the PM_{10} or $PM_{2.5}$ fraction of particulate matter due to their negligible mass. However, recent toxicological and epidemiological studies have shown that (traffic related) ultrafine particles may be more harmful to health (Oberdörster et al., 2005) than the coarser fraction of particles which are low in number but account for most of the mass in the regulated PM_{10} and $PM_{2.5}$ fractions. As a result, there recently has been an increasing interest in modelling the number concentration of ultrafine particles. For an overview the reader is referred to the review articles of Kumar and collaborators (Kumar et al., 2010; Kumar et al., 2011)

In the dispersion modelling of ultrafine particulate matter, it is customary to study the entire size distribution of the UFP number concentration rather than only the total number of particles (based upon a mean particle diameter). In many cases such a size-resolved approach is believed to be necessary in order to appropriately represent ultrafine particles since their dispersion is not only governed by the typical transport processes such as advection and diffusion, but also by a variety of UFP transformation processes such as coagulation, condensation, deposition and nucleation. While the transport processes mainly affect the spatial distribution and the dilution of UFP, the transformation processes (also referred to as particle dynamics) have a direct effect on the shape of the size distribution and the total number of particles. However in the context of urban traffic related UFP dispersion modelling, no consensus has been reached in the literature whether the transformation processes are of enough significance to be included in the modelling or whether they can simply be neglected (Kumar et al., 2010), mainly due to the structural and parametric uncertainty in the existing models (Kumar et al., 2011).

In this work, we present a tool that may be used to investigate this hypothesis. We have developed a computational model that simulates the dispersion and dynamics of ultrafine particles and have applied it to the case of a traffic tunnel. When investigating traffic related UFP and their behaviour in the atmosphere on an urban scale, road tunnels form an interesting environment, both in the perspective of measurements as well as model development and testing. In a traffic tunnel, external factors that influence local air quality are limited or relatively easy to monitor compared to urbanised environments. Such a tunnel environment typically exhibits a uniform quasi one-dimensional wind flow, well mixed concentrations, generally quasi continuous traffic flows, high concentration of pollutants with a large contribution of traffic, and a limited inflow of fresh air. This restricted environmental complexity together with the simple geometry allows for an accurate and fast modelling of traffic emitted pollutants as in principle, the full 3D dispersion model can be reduced to a one-dimensional problem. This makes the model particularly suitable for testing and developing different UFP dynamics models, both in terms of parametrisations as well as numerical representation. This should give us a better insight in the relevant processes that govern the UFP size-distribution in a traffic tunnel, but also more general, within an urban environment.

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DESCRIPTION OF THE UFP TUNNEL MODEL

The model consists of a number of modules that implement the most important transport and transformation processes, i.e. emissions, advection, deposition, coagulation and condensation. An overview of these modules is graphically represented in Figure 1.

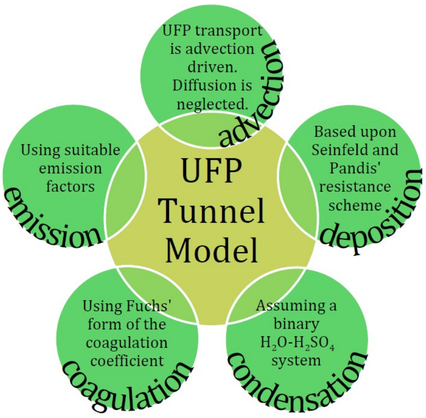


Figure 24. A graphical overview of the different modules in the UFP tunnel model.

The model calculates a continuous UFP number distribution at every location inside the tunnel (assuming a uniform concentration along every cross section). A typical example of the model output is depicted in Figure 2.

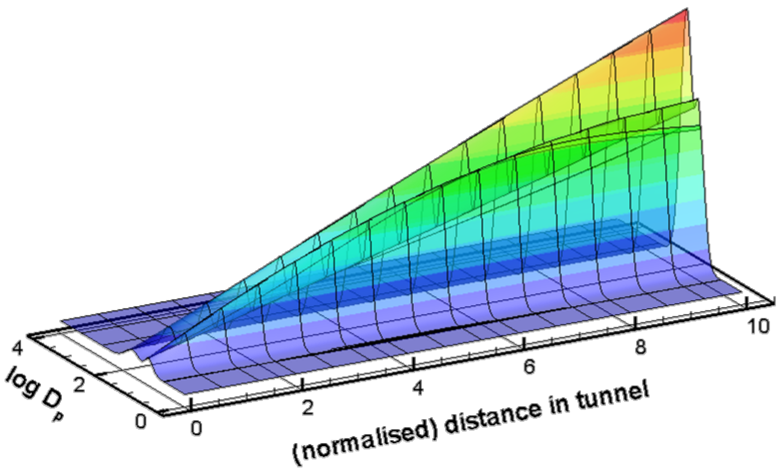


Figure 25. The UFP tunnel model computes the UFP concentration in function of the particle size and the position within the tunnel.

Despite its resemblance with existing aerosol box models and previous UFP tunnel models such as the one proposed by Gidhagen et al. (2003), the presented UFP tunnel model differs in the following sense:

- **A continuous description**
  Most UFP models employ a discrete and rather coarse representation of the solution (e.g. by using a size bin approach) based upon the discrete formulation of the General Dynamic Equation (GDE). We start from the continuous formulation and use corresponding high-accurate numerical methods.
- **High-accurate state-of-the-art numerical methods**
  We have combined the Discontinuous Galerkin method with a high-order finite element approach. Such high-order methods are known to yield high-accurate solutions.
- **A fully size-resolved approach**
  Next to a size-resolved description of the solution, we have also adopted a fully size-dependent description of the various transformation processes. As such, parameters such as the deposition speed, the coagulation coefficient and the condensation are expressed in function of the particle size.
- **A two-dimensional model**
  Aerosol dynamics box-models generally only depend on the particle size. The presented model calculates the UFP concentration in function of the particle size and the (axial) position inside the tunnel. As result, the model can be classified as a wo-dimensional time-dependent model.

VALIDATION UFP TUNNEL MODEL

We have validated our model by means of the results of a recent road-tunnel size-resolved UFP measurement campaign (Cheng et al., 2010) in Taiwan. One of the bottlenecks modelling the dispersion of UFP is the lack of suitable UFP traffic emission data to be used as input for the model. Therefore, we have tried to estimate the UFP emission factors by means of the validation data itself. By using linear regression techniques, we have used the entrance section of the tunnel (a section not significantly affected by the non-linear UFP transformation processes) to estimate the size-resolved UFP emission factors of the passing vehicles. The results are displayed in Figure 3.

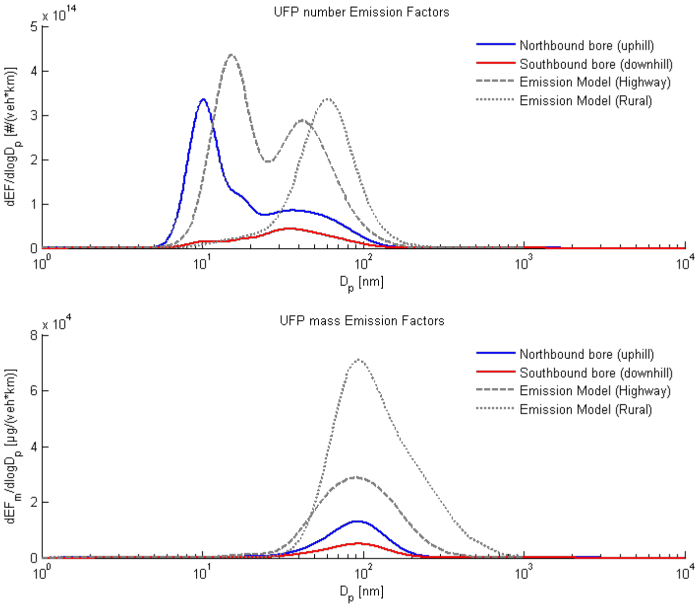


Figure 26. Estimation of the UFP emission factors and comparison with the emission factors of the emission model of Nikolova et al. (2011)

Note that for completeness we have also added the UFP mass emission factors (simply calculated based upon the UFP number emission factors and assuming spherical particles and a constant density) in this figure. In addition, we have also included the emission factors as calculated by the emission model of Nikolova et al. (2011) for comparison.

Running the model based upon these emission factors and configuring it according to the specifications found in the article of Cheng et al. (2010), we can conclude that the model is able to accurately reproduce the evolution of the UFP size-distribution along the length of the tunnel. This can be seen from Figure 4 where the UFP size-distribution after one quarter of tunnel is plotted. There is a good correspondence between the modelled results and the measured data. A similar correspondence has been observed for the entire length of the tunnel.

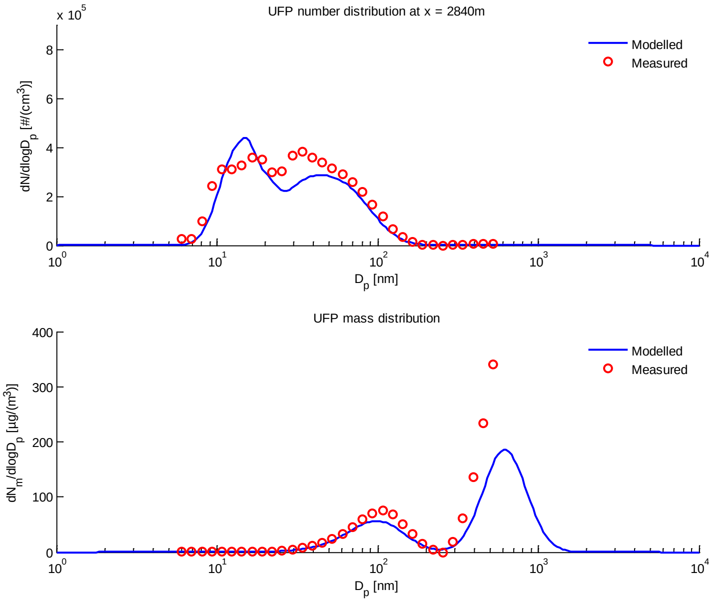


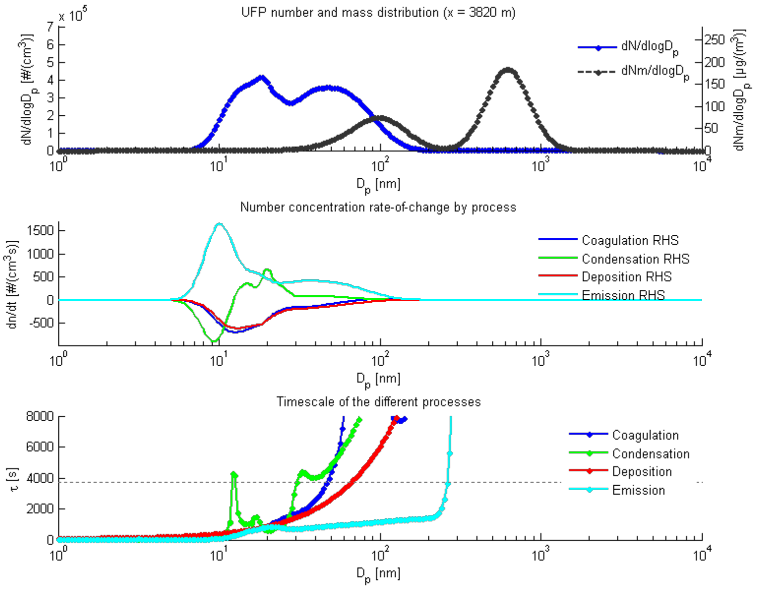
Figure 27. Validation of the tunnel model. Modelled results versus measured data after.

IDENTIFYING THE DOMINANT UFP TRANSFORMATION PROCESSES

A possible approach to quantitatively assess the importance of the different processes is to use a time-scale analysis by investigating the time-scale of each of the processes. The time-scale τ of a process i can be defined as the concentration n divided by the concentration rate-of-change due to the process, i.e.

$$\tau_i = \left| \frac{n}{\left| \frac{\partial n}{\partial t} \right|_i} \right|. \qquad (1)$$

Note that in this work, we would like to propose a size-resolved time-scale analysis. Rather than considering the time-scale of a process for the total number of particles, we will here consider the time-scale in function of the particle size. Although this may seem counterintuitive, this implies that the time-scale of a certain process is identical for both the number and the mass distribution of the UFP concentration. This can be appreciated by the multiplying the denominator and the numerator in Equation by the mass of the particles. An identical time-scale seems to imply that a certain process has a similar effect on both number distribution and mass distribution. However due to the size-resolved approach, the time-scale will also depend on the particle size. But as we can see in figure 4 that the size-range of interest is different for both these distributions, it can be understood that a certain transformation process will have a different impact on the number distribution than on the mass distribution. Figure 5 shows the time-scale of the different processes inside the tunnel after almost 4 km.



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