Dilution and Aerosol Dynamics in a Diesel Car Exhaust Plume – Measurements and Simulations of On-road Conditions

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ABSTRACT:

In this project, the dilution and transformation processes within a passenger car exhaust plume are studied for typical atmospheric and on-road conditions. Particle and exhaust gas measurements within a vehicle exhaust plume were made under real conditions on motorways. Detailed fully coupled CFD / aerosol dynamics simulations have been conducted for H_2SO_4-H_2O-soot aerosol in order to consider several interacting processes.
Particle size distribution measurements at 0.45 m and 0.9 m distance within the exhaust plume indicate a dominant, consistent soot mode at 48 (±3) nm and number concentrations of up to 10^7 cm^{-3} depending on car operating conditions. The test car was run with low sulfur fuel (<10 ppm), and high nucleation particle (Dp≤15 nm) concentrations (>10^7 cm^{-3}) were only recorded under extreme driving conditions such as strong acceleration or high speed (>140km/h) and high rpm (>3800).
The simulations revealed the importance of an accurate description of turbulent species and transport. In particular, turbulent diffusion of soot mode particles is attributable for the measured decrease of soot mode number concentrations within the exhaust plume. The simulations showed a strong sensitivity to fuel sulfur content and/or sulfur to sulfate conversion. The simulated growth of H_2SO_4-H_2O nucleation particles was insufficiently low to explain measured nucleation particle concentrations due to the detection limit of the SMPS system. Simulations with simplified condensable hydrocarbons resulted in faster and sufficient growth of nucleation particles.

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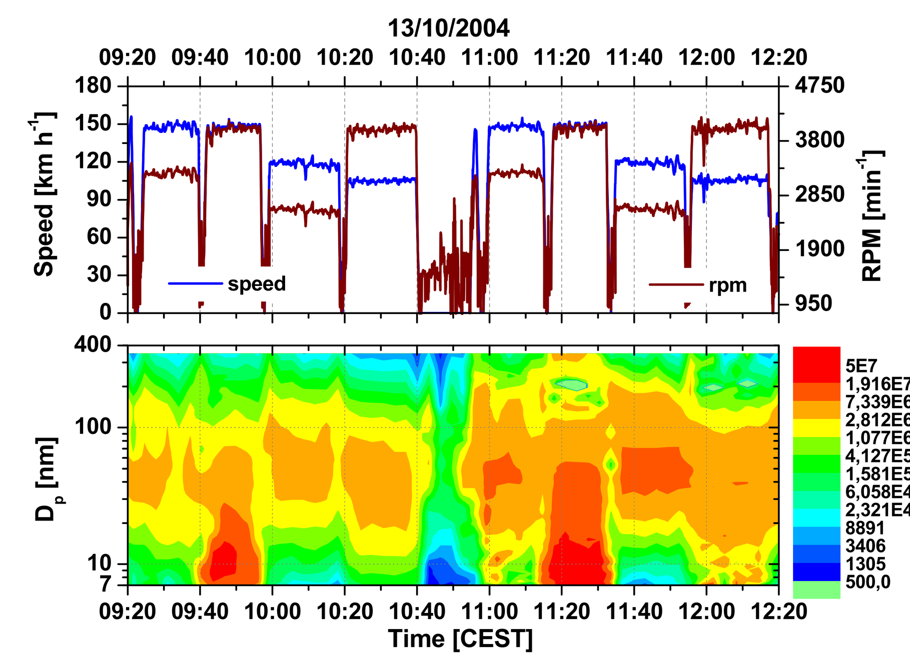
Introduction

Inlet system used in this project: SMPS, exhaust gas, humidity, temperature and flow velocity measurements are taken at adjustable locations within the exhaust plume on public roads

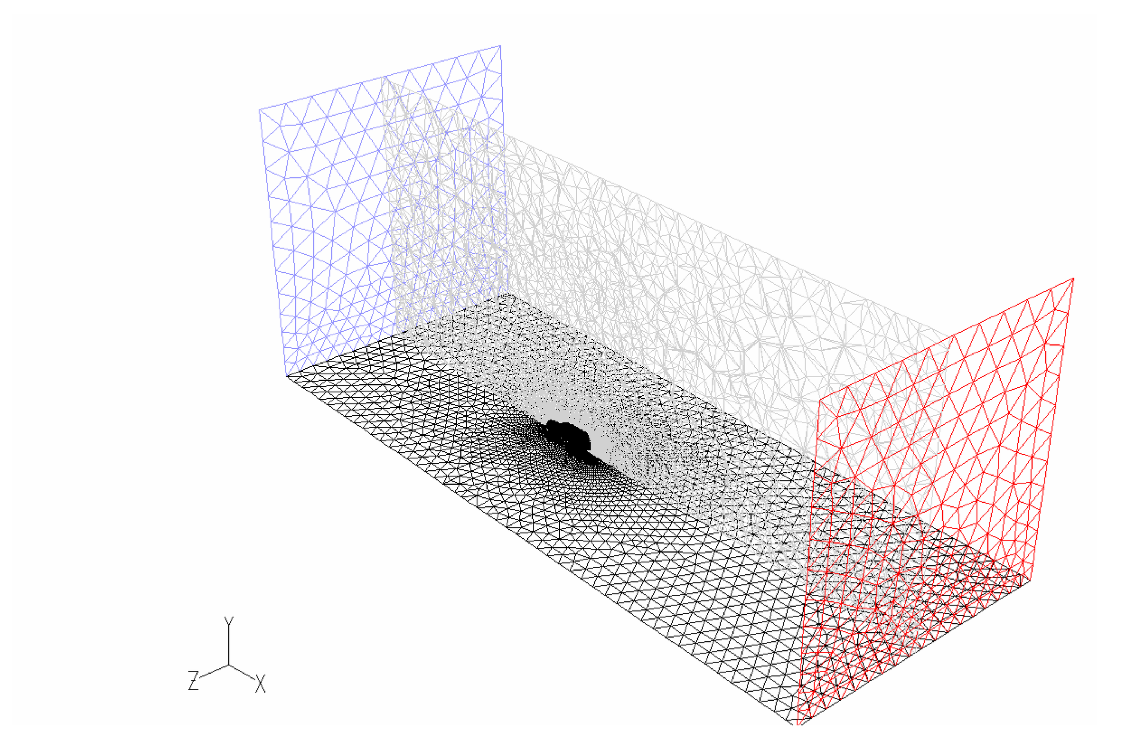
- Adverse health effects associated with respirable ultrafine particles emitted from vehicle exhaust
- Main sources of ultrafine particles (d_p < 100 nm) are Diesel vehicles
- Aim of this project:
  - How do particle sizes distributions look like within the car exhaust plume under real atmospheric and on-road conditions?
  - Where do particles < 10 nm form?
  - Impact of rapid turbulent exhaust dilution on growth and nucleation
  - Combined approach by measurements and coupled CFD/Aerosol model



Measured vehicle speed and rpm (top), and size distribution (bottom) on 13 October 2004)

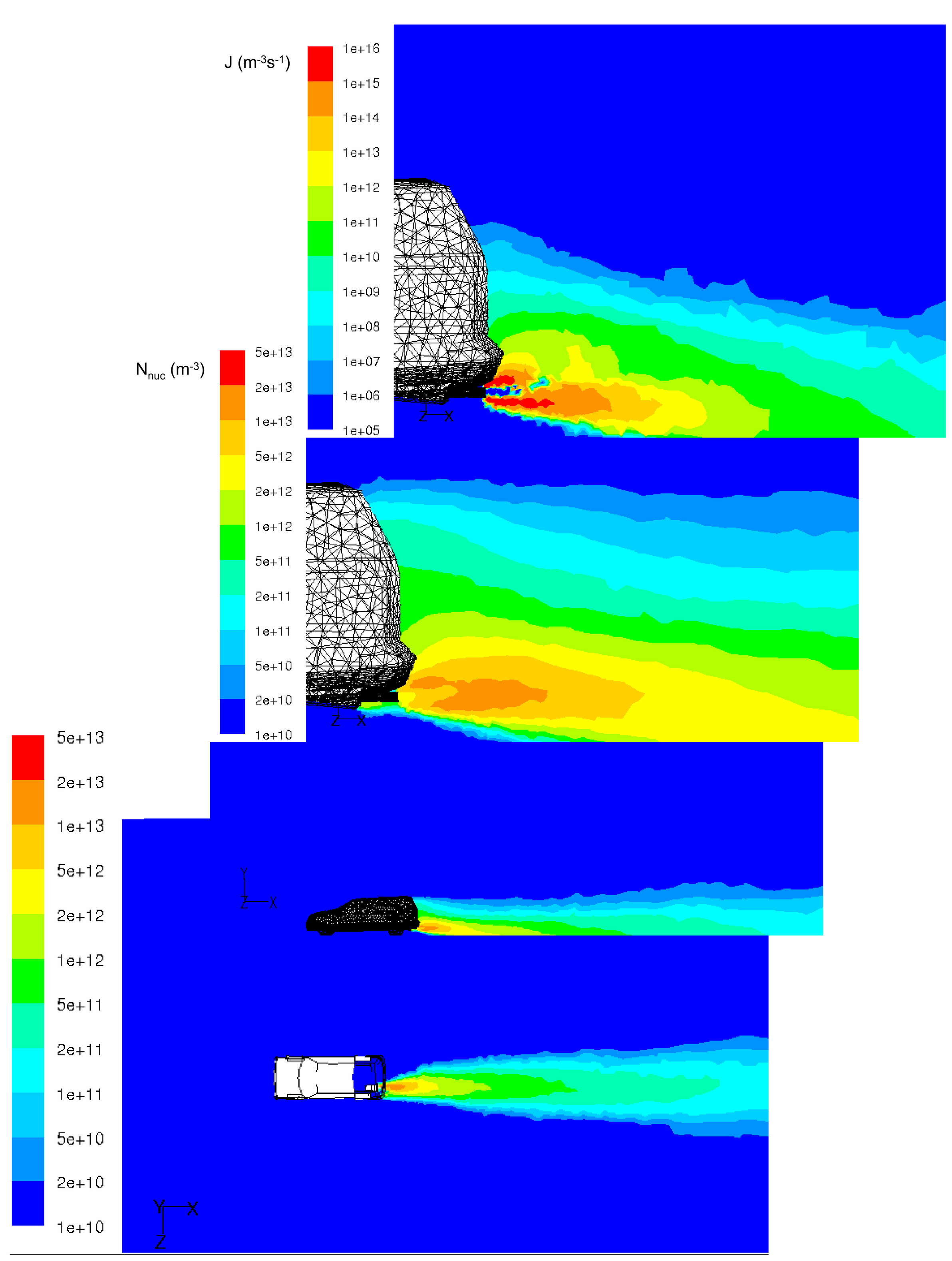
Modelling Approach

- Creation car geometry / numerical mesh in "computational wind tunnel"
- CFD simulations using FLUENT 6 (www.fluent.com) for flow exhaust gases and verification (resolution, trace gas measurement)
- Add-on FPM (Fine Particle Model, www.particle-dynamics.de) enables computation of aerosol dynamics and particle dispersion coupled with flow
  - Euler-Euler solution technique
  - Utilizes the method of moments together with the modal assumption
- Extension FPM by user defined functions to calculate H_2SO_4-H_2O nucleation and growth
- Development of a parameterization for particle composition (H. Vehkamäki)
- Further extension to assess growth by low-volatile HC



- Focus of the modelling effort: exhaust region, body simplified, 260000 grid cells
- Turbulence: k-ε closure
- Soot-H_2SO_4-H_2O aerosol particles (core-mantle)
- Boundary conditions for simulations are based on fuel consumption and composition, vehicle speed, air mass flow, air/fuel-ratio, exhaust-T measurements and ambient conditions
- Free parameters:
  - Prescribed exhaust soot mode particle flux adjusted to fit measurements at 0.45 m and 0.9 m
  - Exhaust $H_2SO_{4(g)}$ → sensitivity studies based on fuel sulphur content (FSC) and SO_2 to SO_3 conversion

Results:

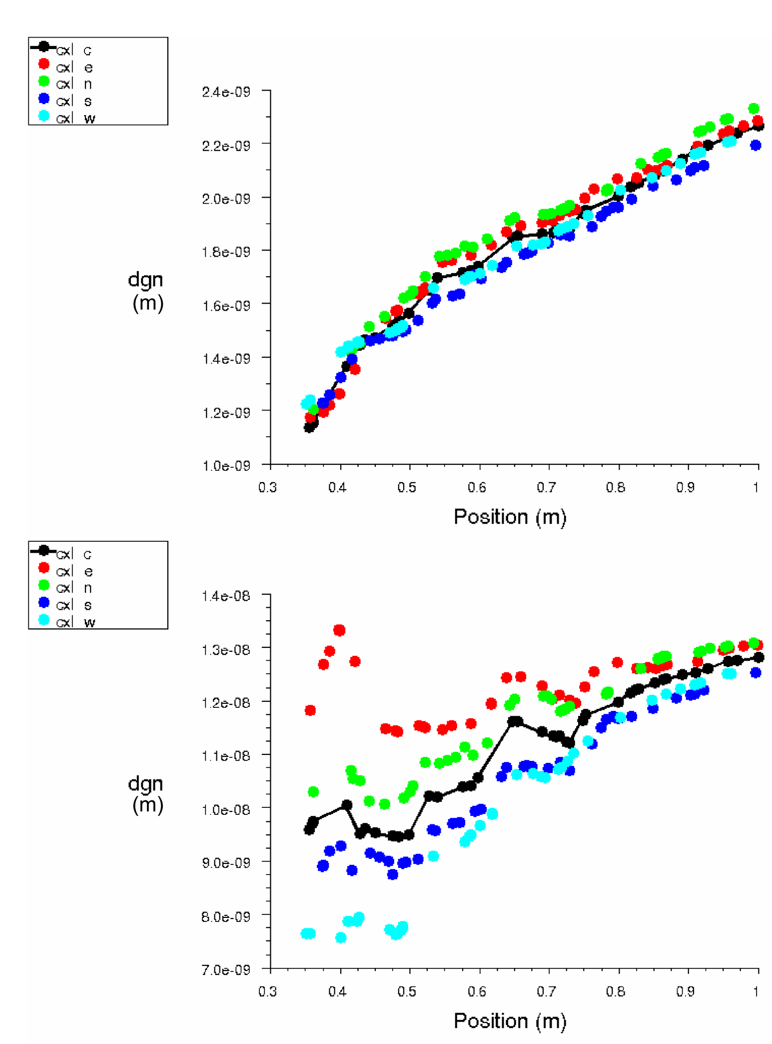


Cross sections exhaust pipe centre planes simulated N_{nuc} (2 bottom panels) and close-up near exhaust region (lower top) in $\#m^{-3}$ and nucleation rate (top) in $\# m^{-3}s^{-1}$ for 145 km/h, mass flow rate 0.08 kgs^{-1}, prescribed soot mode particle flux 10^{13} s^{-1} ($2.6\cdot10^{14}$ $\#km^{-1}$)

V km/h	rpm min^{-1}	N_{nuc} cm^{-3}	d_{g-nuc} nm	σ_{nuc}	N_{soot} cm^{-3}	d_{g-soot} nm	σ_{soot}
148	3240	1e6	10	1.3	8e6	48	1.9
		-	-	-	3e6	52	1.7
148	4020	5e7	6	1.9	1e7	44	1.8
		2e7	11	1.5	5e6	45	1.6

Table: Data sampled at 0.45 m (blue) and 0.9 m (black) centreline distance behind exhaust pipe. Mean values obtained by fitting SMPS size distributions to a log-normal form from 10 scans

- **Measurements (FSC < 10 ppm, 2l/ 74KW Euro 3 Diesel engine)**
  - **N_{soot} dominated measured size distribution under most driving conditions up to $10^7 cm^{-3}$**
  - **high N_{nuc} (> $10^7 cm^{-3}$) only measured at V > 140km/h & > 3500 rpm**
- **Simulations**
  - **Strong sensitivity towards $H_2SO_{4(g)}$-flux**
  - **Location of highest nucleation rates where gradients of T, RH and H_2SO_4 are strongest**
  - **$9\cdot10^{-7}$ mol/s exhaust $H_2SO_{4(g)}$ → N_{nuc} > $10^7 cm^{-3}$ good agreement in N pattern with measurements (corresponds to a FSC of 350 ppm & S→SO3 conv. rate of 0.03 / FSC of 10 ppm and a conv. rate of 1) → effect of S storage effects on catalyst, lube oil S & purging?**
  - **Growth H_2SO_4-H_2O nucleation mode particles insufficiently low, growth of soot-H_2SO_4-H_2O particles insignificant → additional low volatile HC (simplified) leads to sufficient growth (nucleation mode up to 15 nm)**



Simulated d_g in m near exhaust plume region for nucleation particles consisting of H_2SO_4-H_2O (top) and simplified H_2SO_4-H_2O-HC, cxl-c is the centreline of the exhaust pipe, cxl-w, cxl-e, cxl-n, and cxl-s are shifted 2 cm to the left, right, upward and downward. Measured fitted values at 0.45 m: 6-10 nm, at 0.9 m: 11-16 nm