## 11<sup>th</sup> ETH-Conference on Combustion Generated Nanoparticles August 13<sup>th</sup> –15<sup>th</sup> 2007

### **Application Form**

X I am planning to **attend the meeting** on  $13^{th} - 15^{th}$  of August 2007 at ETH Zurich

<ul><li>I will attend the dinner party on Monda</li><li>I will attend the welcome party on Sun</li></ul>	, ,			
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### 11<sup>th</sup> ETH-Conference on Combustion Generated Nanoparticles August 13<sup>th</sup> -15<sup>th</sup> 2007

### Paper/Poster-Abstract Form

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**Title:** 1D Dynamics of Car Exhaust Particles

Abstract: (min. 300 - max 500 words)

We studied the particle dynamics of light-duty diesel engine exhaust particles in the VELA-2 laboratory facilities (JRC, Italy) both by experimental measurements and modelling. The experimental setup consisted of a long flexible cylindrical tube (informally called anaconda) connected to the car exhaust pipe (TP) that transferred the exhaust fumes into a wider cylindrical duct (dilution tunnel-DT) where they were diluted with filtered dilution air. The walls of the anaconda were kept at a constant temperature of 70°C, whereas a constant room temperature was assumed for those of the DT. For simplicity, the experimental manifold was modelled as axisymmetric (the anaconda had a bent with a large curvature radius before reaching the DT). We also measured temperatures and particle number-size distributions at different radial penetrations and axial positions from the TP to the normal Particulate Matter sampling point (SP) in order to investigate the role of potential inhomogeneities.

The results showed that while the dilution air and the exhaust flow rates were approximately constant, strong temperature gradients were often measured close to the walls. The experimental particle size distributions showed only the accumulation mode: the fitted mean mobility diameter evolved from about 70 nm at the TP to 85-90nm at the end of the anaconda with a standard deviation of a few nm. Little evolution of the distribution was instead generally observed within the DT, especially in the case of high dilution ratios.

Analytical considerations and numerical simulations of the fluid flow led to an estimate of the Stokes number of these soot particles St~0.0001, i.e. particles could be treated as passive scalars.

At this stage we focus on a 1D treatment of the car exhaust particle dynamics along the anaconda. We considered agglomeration, described by Smoluchowski equation, as the main mechanism determining particle dynamics. The contribution of turbulence to collisions was neglected since Saffman and Turner kernel for turbulent collisions was estimated as several orders of magnitude below the one for Brownian collisions (see Seinfeld & Pandis). The concept of fractal dimension for the soot aggregates was employed as in Maricq and the fractal dimension was determined self-consistently. The mean diameter of the soot particles was comparable to the mean-free path of the carrier flow and particles found themselves at the crossover between the continuum and free molecular regime.

Fuchs approximation was used to interpolate the kernel between the continuum and the free molecular regime. Diffusional and thermophoretic losses are modelled by extra linear terms added to Smoluchowski equations and the deposition coefficients are estimated by means of 1D correlations (see Voutisis et. al.).

Solutions of Smoluchowski equation were first obtained with a sectional method employing a large (~6000) number of evenly spaced bins.

Subsequently, the algorithm was significantly improved by using a logarithmically-spaced grid allowing one to reach a similar accuracy with 100 bins, thus significantly reducing the computational time.

In the future, we plan to include explicitly the effect of particle convection in the study of particle dynamics.

#### References:

Voutsis E., Ntziachristos L. & Samaras Z. (2005), *Atmospheric Environment*, 39, 304-318. Maricq M. (2007), *Aerosol Science*, 38, 141-156.

Seinfeld J.H. & Pandis S.N. (1998), Atmoshperic Chemistry and Physics, John Wiley & Sons.

### Short CV:

Lorenzo Isella graduated in Physics from the University of Pavia in 2001. He holds a Ph.D. in Physics awarded by the University of Hertfordshire (United Kingdom) in 2005. He worked for a few months as junior business analyst in Banca MB, Milan. He is currently a research fellow at the European Commission – DG Joint Research Centre, Institute for Environment and Sustainability, Ispra, performing modeling work to support the activities in the Vehicle Emission Laboratory (VELA).

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# 1D Dynamics of Car Exhaust Particles

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### Introduction

We develop a 1D treatment of light-duty engine exhaust particles along the tube leading the fumes from the tailpipe to the inlet of the dilution tunnel. Agglomeration, diffusional and thermophoretic losses are accounted for. Inertial deposition is neglected due to the low particle Stokes number.

# 1D Description

Simplification of GDE for steady-state condition and moderate Reynolds numbers:

$$\frac{\partial n_q}{\partial t} + U \frac{\partial n_q}{\partial x} = \mathcal{D}_q \frac{\partial^2 n_q}{\partial x^2} + \omega_q$$

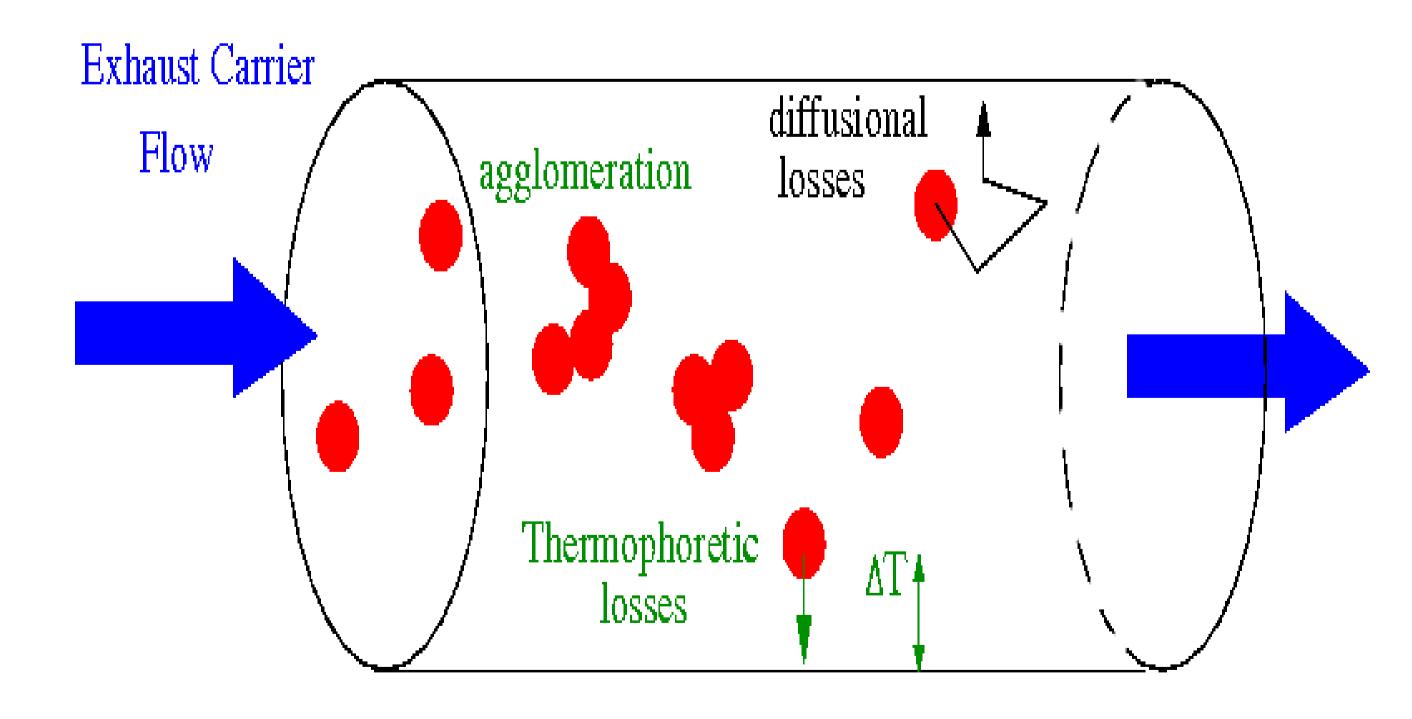
Steady State

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Convection dominant over diffusion

$$x = U\tau \longrightarrow \frac{\partial n_q(U\tau)}{\partial \tau} = \omega_q(U\tau)$$

$$\omega_{q} = \frac{1}{2} \sum_{i,j}^{N_{b}} \chi_{ijq} \mathcal{K}_{ij} n_{i} n_{j} - \sum_{i}^{N_{b}} \mathcal{K}_{iq} n_{i} n_{q} - \gamma_{\text{dif}} n_{q} - \gamma_{\text{th}} n_{q}$$
Coagulation diffusional thermophoretic losses



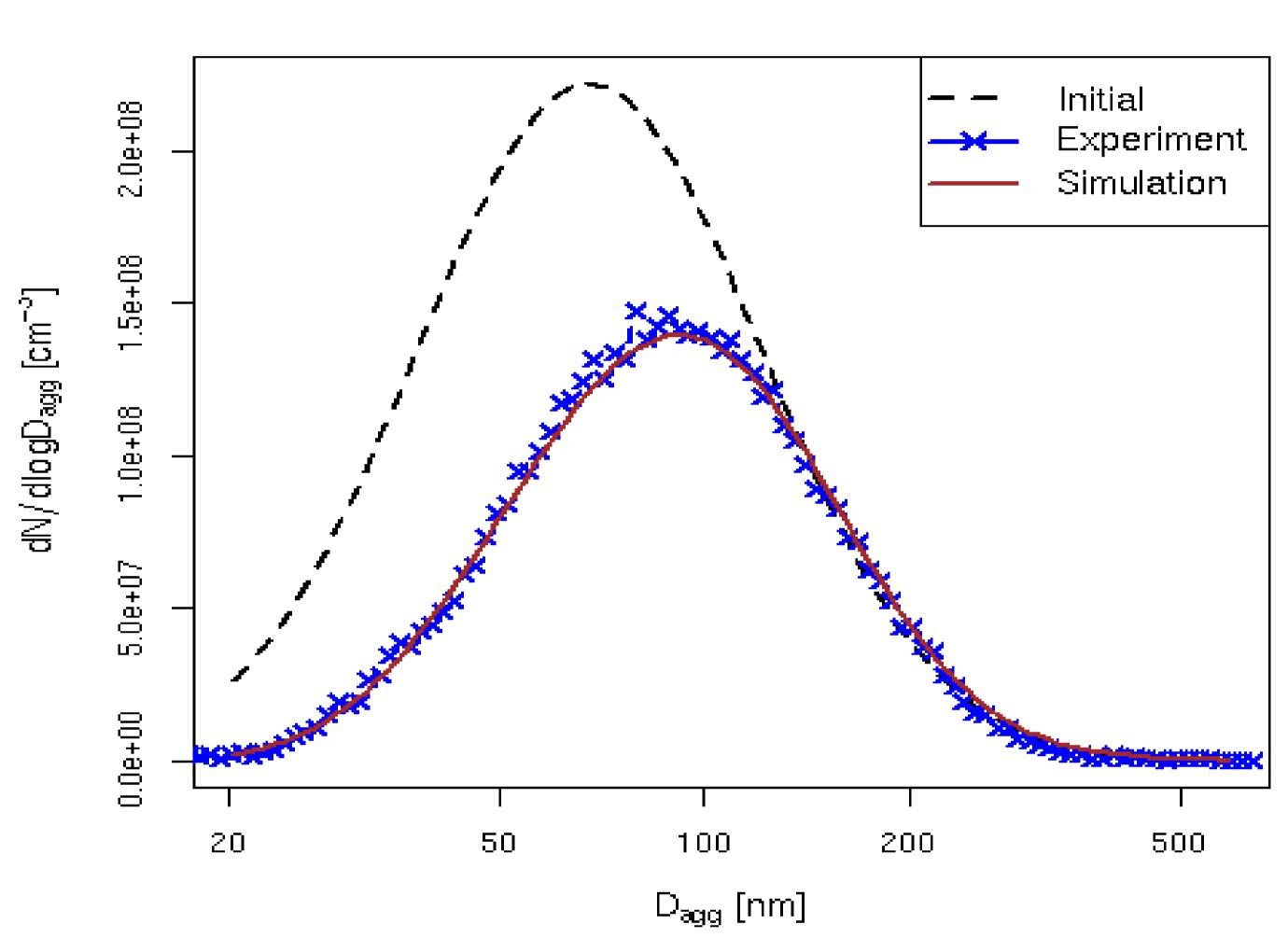
Numerical Solution of the GDE (Smoluchowski equation in residence time)

- •Discretization of particle distribution on a 100-channel grid.
- •Sectional Method and system of ODE's.
- •Accuracy of the simulation checked by ensuring mass conservation in the absence of particle losses.
- •Aggregate fractal dimension assumed constant and determined self-consistently.

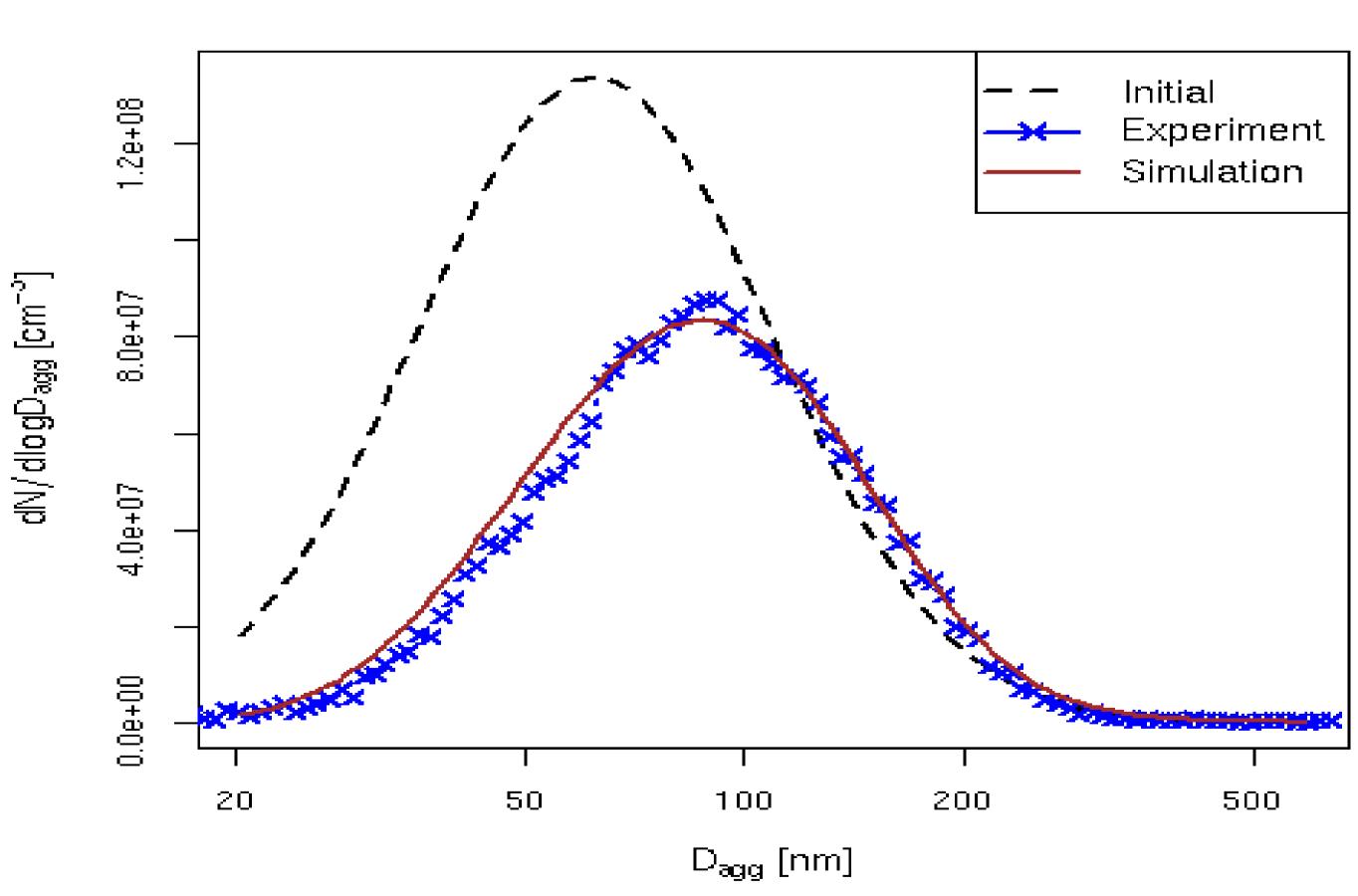
# Experiments at JRC VELA-2 and Numerical Simulations

- •Car speeds 120 and 50Km/h.
- •Solid particle number-size distributions measured with SMPS.
- •Residence times about 2 and 4.5 seconds, respectively.
- •Determined fractal dimensions 2.25 and 2.1, respectively, for assumed primary size 20nm.

Car speed 120Km/h



Car speed 50Km/h



## **Conclusions and Recommendations**

- Dynamics dominated by coagulation.
- Strong influence of fractal dimension on aerosol dynamics.
- •Thermophoretic losses about 5-7%  $\rightarrow$  resuspension of deposited material.
- •Particle residence time can affect the measurement at the sampling point when the distribution "freezes" in the dilution tunnel (e.g. for high dilution ratios).
- •Indirect estimate of the importance of condensation.

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