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High-Accuracy Nanoparticle Sensor for Combustion Engine Exhaust Gases

M. Kraft^{a,*}, J. Kaczynski^a, T. Reinisch^b, M. Unger^b, A. Bergmann^{b,c}^aCTR Carinthian Tech Research AG, Europastraße 12, 9524 Villach, Austria^bAVL List GmbH, Hans-List-Platz 1, 8020 Graz, Austria^cInstitute of Electronic Sensor Systems, Graz University of Technology, Inffeldgasse 10/II, 8010 Graz, Austria

Abstract

Nanoparticles are one indispensable analyte in the characterisation of any combustion engine or exhaust aftertreatment system. To improve the presently prevalently used condensation nucleus magnification-based particle counters (CNC) in performance and footprint, a dedicated, comprehensive all-in-one CFD model was developed. Following experimental validation, the model was successfully used to simulate and better comprehend the internal functionalities of the present standard system, identify critical design parameters and develop a new, improved sensor system design. The ensuing improved CNC nanoparticle sensor is now based on a vertical, annular design. Besides being highly compact, the new layout yields an almost perfectly homogenous (super-)saturation of the aerosol stream and superior temperature control of all relevant components. This gives the new design a uniquely high discriminatory power by nanoparticle diameter, a precise controllability of the effective particle detection cut-on size and a significant reduction in the effective particle losses in the sensor.

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1. Introduction

Among the various airborne pollutants, in particular nanoparticles < 100 nm are presently regarded with increasing concern. As internal combustion engines in general – and Diesel engines in particular – are one relevant

* Corresponding author. Tel.: +43 4242 56300; fax: +43 4242 56300 400.

E-mail address: martin.kraft@ctr.at

particle source, the particle emission is a parameter that has to be reliably and efficiently measured [1]. Similarly, the efficiency and effectiveness of exhaust aftertreatment systems, like (nano-)particle filters has to be controlled. The present, legally mandated standard measurand for the analysis of such automotive exhausts is the particle number concentration, i.e. the actual count of nanoparticles ≥ 23 nm per time unit. As these particles are way too small for a direct, individual detection e.g. by optical means, the standard approach is to exploit the condensation nucleus magnification principle to build a condensation nucleus counter (CNC). The aerosol stream is first saturated with working fluid vapours, typically n-butanol, and then cooled down to achieve a super-saturated atmosphere. Under these conditions, the nanoparticles may act as condensation nuclei, i.e. working fluid condenses on them and grows them to typically μm -sized particles that can then easily be counted [2]. The critical particle diameter d_K above which this happens can be derived from the Kelvin equation according to

$$d_K = \frac{4 \cdot \sigma \cdot M}{\rho \cdot R \cdot T \cdot \ln S} \quad (1)$$

The cut-on size of the detection method thus depends on *i*) the material properties of the working fluid, in particular its liquid density ρ , surface tension σ and molar mass M , and *ii*) the temperature T and gas (super-) saturation S near the particle. CNC-based particle sensing thus depends on carefully balanced processes to achieve reliable, reproducible particle detection. The increasing demand for ever more precise and reliable sensors and smaller footprints now calls for new, integrated approaches. For this reason, in a first step a comprehensive, dedicated in-depth simulation model of a CNC sensor was developed, implemented and validated for an established, routinely used CNC device.

2. Nanoparticle Sensor Modelling

2.1. Sensor Simulation Model

The entire sensor simulation model was established in ANSYS-Fluent. Each simulation was based on a detailed 3D geometry model of the respective CNC sensor. The flowing medium was modelled as air using the standard Fluent model; for all other gaseous, liquid or solid components, all relevant parameters were modelled as polynomial functions of temperature for the range 10 – 90°C, based on literature data. Regarding the working fluid n-butanol, this included gas and liquid density, vapour pressure, surface tension, gas viscosity, gas heat capacity, gas thermal conductivity, evaporation enthalpy and the binary diffusion coefficient in air. Air – working fluid mixtures were modelled using the ideal gas approximations in Fluent. All solid parts, i.e. Al for the structural parts and the respective polymers for the thermal insulation elements separating the different temperature zones and the saturator element, were defined by their material density, heat capacity and thermal conductivity. The set temperatures were defined at the outer surfaces of the aluminium structural blocks. All gas – solid interfaces in the saturator and downstream of it were modelled as working fluid vapour equilibrium sources / drains, as defined by the surface temperature and the related working fluid vapour pressure. The simulation model thus accounts for the gas flow, heat exchanges between and resulting thermal distributions in all solids and the gas phase, the evaporation and subsequent distribution of n-butanol, and its super-saturation in the condenser zone of the CNC. The Kelvin diameter distribution is then calculated from these values in post-processing using Eq. 1.

A key simplification made was modelling the aerosol particles as mass-less flow trajectories evenly spaced across the gas inlet, rather than individual items. This assumption was validated by separate simulations using two-phase discrete particle models, in particular the Stokes-Cunningham approach for sub-micron particles. These simulations showed that the reciprocal effect of the presence of solid nano-particles, and later of liquid micro-droplets, on the flow regime is negligible for the particle volumes occurring in a CNC sensor. However, the work also showed that the approximation becomes increasingly unreliable for even smaller nano-particles ≤ 12 nm. While not affecting the flow, for this particle size range enhanced simulations models – and probably a fundamentally different CNC sensor layout – would be required.

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