PEMs4Nano

Portable Nano-Particle Emission Measurement System

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Written By	Jethro Akroyd (UCAM)	
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Publishable Executive Summary

The work presented in this report is part of a project to develop devices and procedures to measure particles down to 10 nm in size emitted from vehicles equipped with gasoline direct injection (GDI) engines. The project entails developing a fundamental understanding of the formation of the particles in the engine, the evolution of the particles as they pass through the exhaust system to the tail pipe of the vehicle, and then as the particles pass through the sample system into the measurement device. This report focuses on aspects of modelling the system used to sample the exhaust from a single-cylinder GDI test engine, and on modelling a gasoline particulate filter (GPF) used to filter particles out of the exhaust from a multi-cylinder GDI test engine. The robustness and application of the models is demonstrated through sensitivity studies.

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1 Introduction

The report presents aspects of work to develop a model of the system used to sample particles down to 10 nm in size from the exhaust of a gasoline direct injection (GDI) engine, and a model of a gasoline particulate filter (GPF) used to filter the exhaust from gasoline engines.

Parametric and sensitivity analysis are crucial steps in the development of the models. These allow identification of the most important model parameters and are often used to support the calibration of a model. Once a model is calibrated, sensitivity analysis can be used to give insight into how the physical system would respond to changes in process conditions and design choices.

In this report, sensitivity analyses are demonstrated for the sample system and gasoline particulate filter models. In the case of the sample system model, sensitivity analysis used to investigate the effect of sample dilution when measuring the particles emitted from a single-cylinder GDI test engine. In the case of the GPF model, sensitivity analysis was used to support the interpretation of experimental data from a multi-cylinder GDI test engine.

2 Sampling process for measurements of particulate emissions

Particulate emissions from engines are largely composed of soot particles formed by incomplete combustion. In addition, vehicle exhaust often contains soluble organic fractions (SOF). The soluble organic fractions are mainly composed of semi-volatile hydrocarbons that condense when the exhaust cools down. When the exhaust is analysed to measure the particulate emissions there is a risk of SOF condensing on the soot particles or even forming new particles composed entirely of SOF. Based on the evidence in the scientific literature [1], it is very likely that SOF condensation preferentially effects small particles, including those in the 10 nm size range that are the focus of this project. For this reason, SOF can introduce considerable errors when trying to measure particulate emissions. The measurement of particulate emissions requires careful dilution of the exhaust to simultaneously reduce its temperature to the operating temperature of the instrument whilst minimizing the effect of the SOF.

In Deliverable D3.2 (SRM Engine Suite for ICE configurations), a Dekati FPS 4000 diluter with two dilution stages (Figure 1) was modelled using a simple network model (Figure 2). The model describes the evolution of particles and condensation of SOF in exhaust sampled from an engine as the exhaust passes through the dilution system into an Engine Exhaust Particle Sizer (EEPS). The control volumes in the network model are specified as constant volume reactors with volumes equal to the physical volume of the piping connections. The first connection (C1) specifies a boundary condition for the temperature, mass flow rate and major species composition of the gas entering the dilution system, in addition to the size distribution and number concentration of the particles carried in the gas. The first reactor (R1) describes the first dilution stage assuming a length 40 mm and diameter of 6 mm. Connections C2 and C5 describe the first and second stage dilution air flow respectively and are specified in terms of the mass flow rate, temperature and major species composition of the dilution air. The second reactor (R2) describes the piping between the first and second dilution stages with a length of 140 mm and diameter of 6 mm. The third reactor (R3) describes the second dilution stage with the same physical dimensions as R1. Finally, the fourth reactor (R4) describes the piping for the second dilution stage to the EEPS. The overall dilution factor in the model is 30 (on a mass basis).

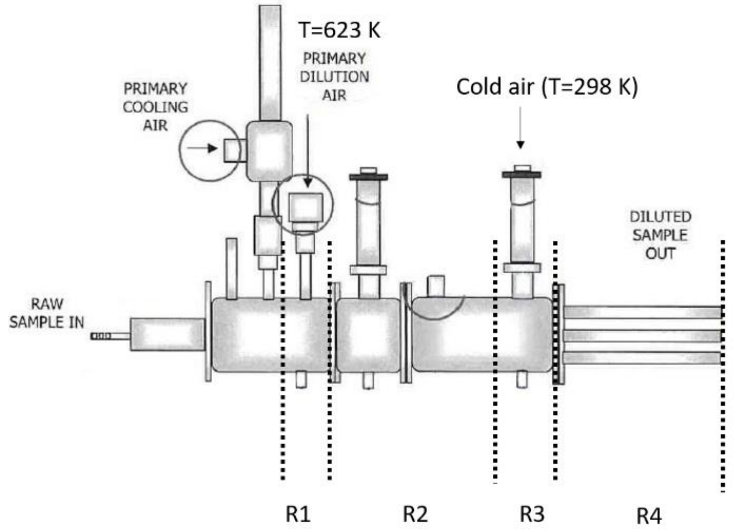

Figure 1: Schematic of the Dekati FPS-4000 that is installed between the engine and the EEPS.

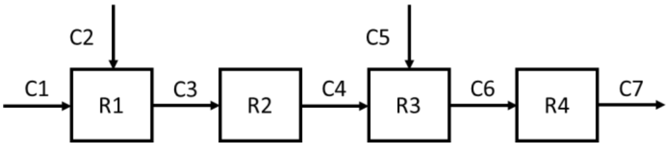

Figure 2: Network model of the sample system.

A sensitivity analyses was performed using the network model shown in Figure 2, including analysis of the sensitivity of the SOF mass fraction as a function of dilution ratio. The results of the SOF sensitivity analysis are shown in Figure 3. The results are able to be used to support the design of the experimental setup.

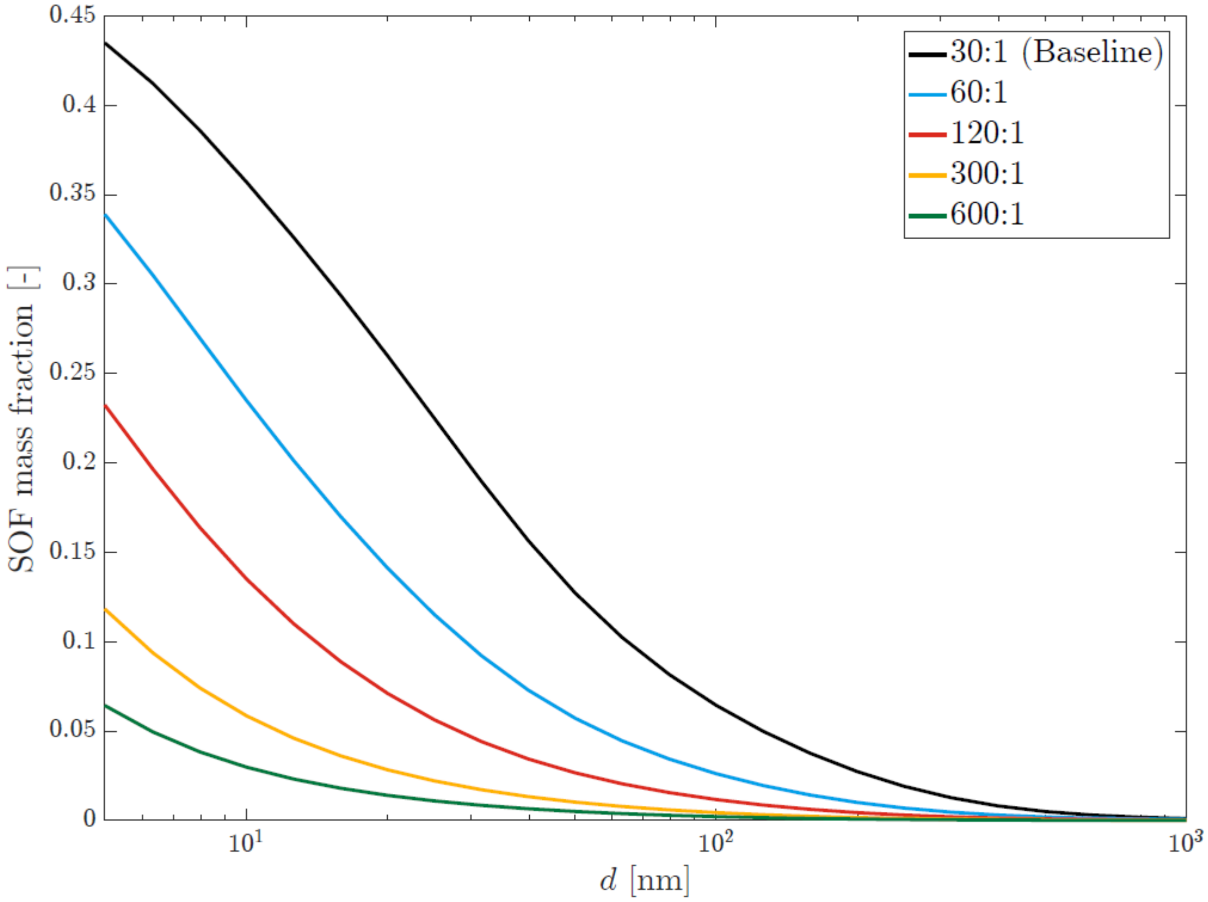

Figure 3: SOF mass fraction entering the EEPS as a function of dilution ratio in the sample system.

3.1 Extension of the sampling process to include a thermal denuder

A thermal denuder and an additional single-stage Dekati ejector diluter were added after the Dekati FPS-4000 to provide assurance that the sample system removes any remaining SOF condensates. The thermal denuder is shown with and without its heating element in Figure 4 and Figure 5 respectively. The single-stage Dekati ejector diluter is present to the right of the denuder.

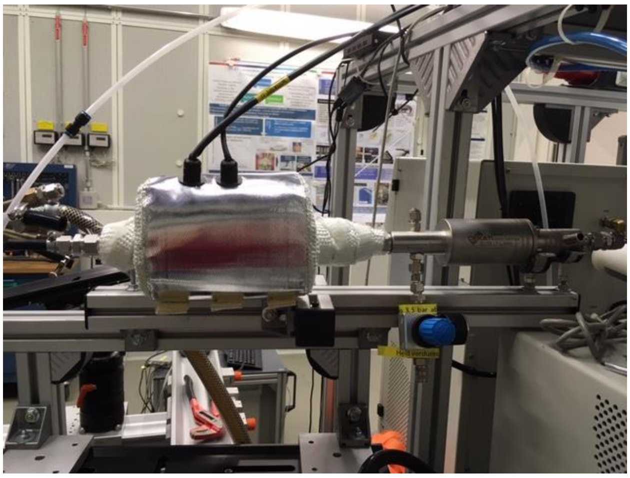

Figure 4: Denuder with the heating element.

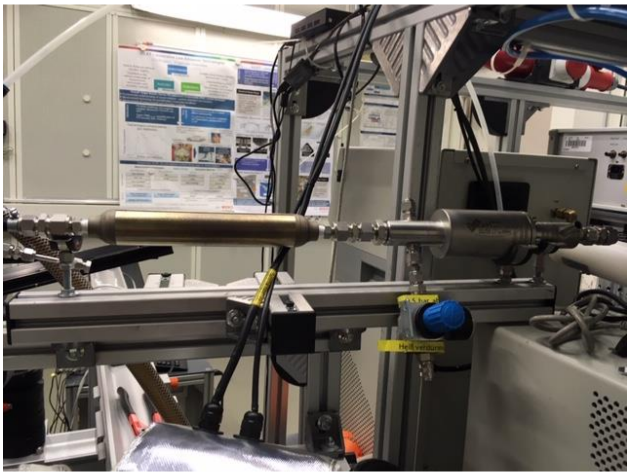

Figure 5: Denuder without the heating element.

The network model developed in deliverable D3.2 (SRM Engine Suite for ICE configurations) was modified to add two additional reactors to represent the thermal denuder (R5) operating at 330°C and the additional diluter (R6), providing a further 10-fold dilution. The modified model is shown in Figure 6.

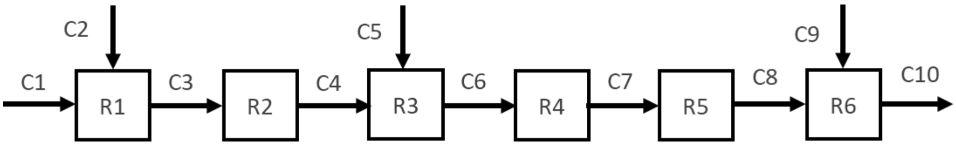

Figure 6: Network model of the sample system with thermal denuder and additional diluter.

The performance of the sample system was investigated experimentally. The particle size distributions from a single-cylinder GDI test engine running at 12 different engine operating points were measured using the EEPS with the original and with the modified sample systems. Each size distribution was measured for approximately 10 minutes at 1 Hz. The distributions measured for the operating points at 1200 rpm are shown in Figure 7. The data are corrected for the dilution in the sample system, such that numbers in Figure 7 correspond to the number concentration of particles in the engine exhaust (i.e. at the point at which it leaves the engine). The data appear to show an increase in the number concentration when using the modified sample system. However, the addition of the thermal denuder should result in more particle losses, not more particles. The apparent increase shown in Figure 7 is not real, but is indicative of the intrinsic difficulty of measuring absolute number concentrations and is well within the expected bounds. The data also show quite significant time fluctuations, which make it difficult to determine the extent to which the thermal denuder changes the shape of the particle size distribution in this case.

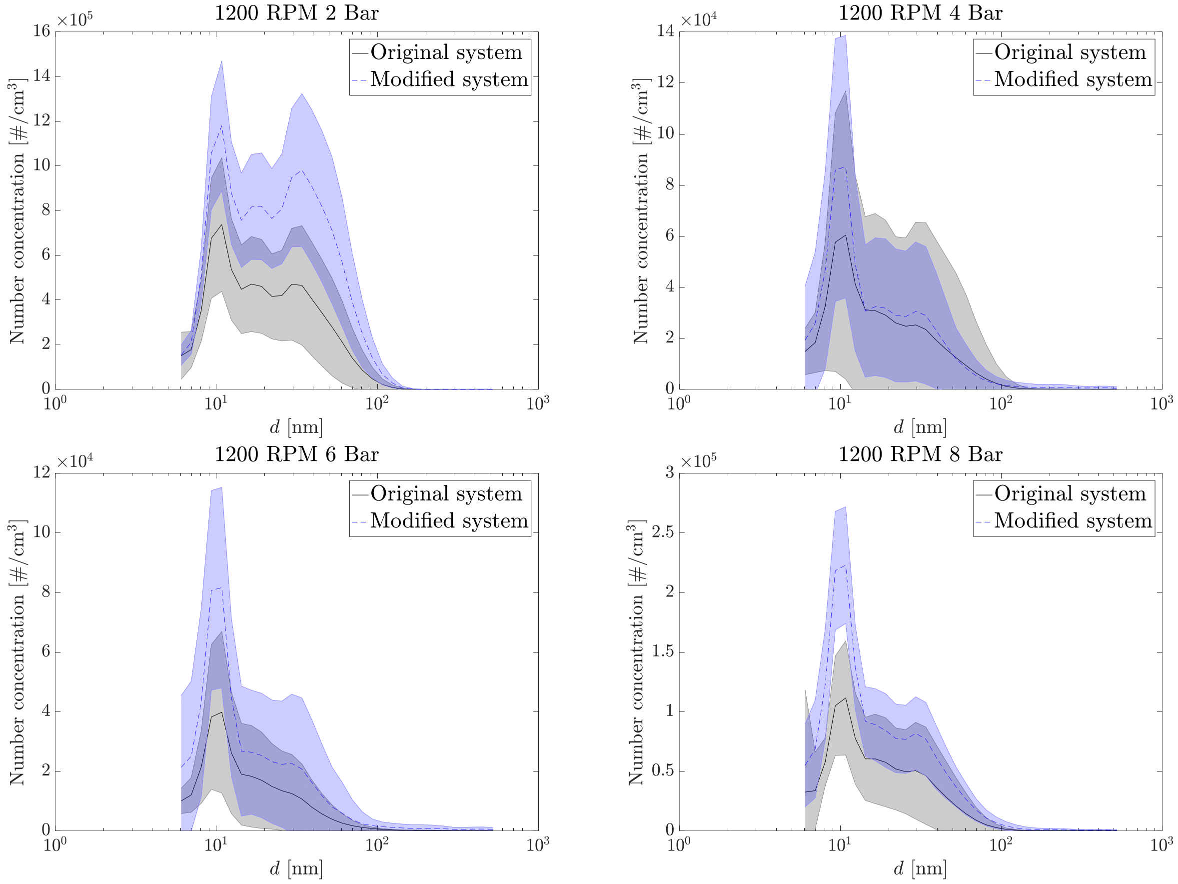

Figure 7: Particle size distributions measured at 1200 RPM. The lines show the time-average of the measured distributions. The shaded regions show a ±1 standard deviation range around the time-average distributions.

The updated network model was used to simulate the evolution of particles and condensation of SOF in the exhaust sampled using the original and the modified sample systems. The simulated SOF fraction is shown in Figure 8. The change in SOF fraction is due to the additional dilution. Given the extent of the uncertainty due to the fluctuations in the experimental data, the effect of the thermal denuder on the shape of the particle size distribution was not considered here.

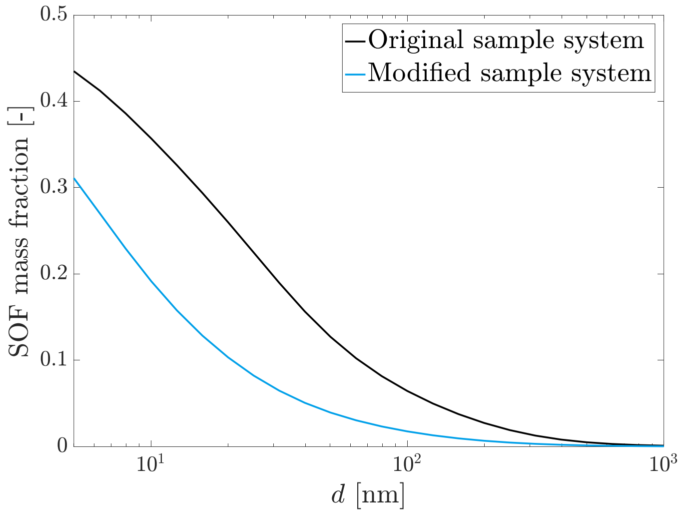

Figure 8: Reduction in SOF mass fraction in the original and modified sample systems.

3 Gasoline particulate filter model

The particulate filters used in exhaust aftertreatment systems are based on wall flow monolith devices. The structure of a typical device is illustrated in Figure 9. The device consists of a set of channels separated by porous walls. Alternate channels are open only at the inlet or outlet side of the device. The only way that gas is able to pass through the device is by flowing through the porous walls, which act to filter particles out of the exhaust.

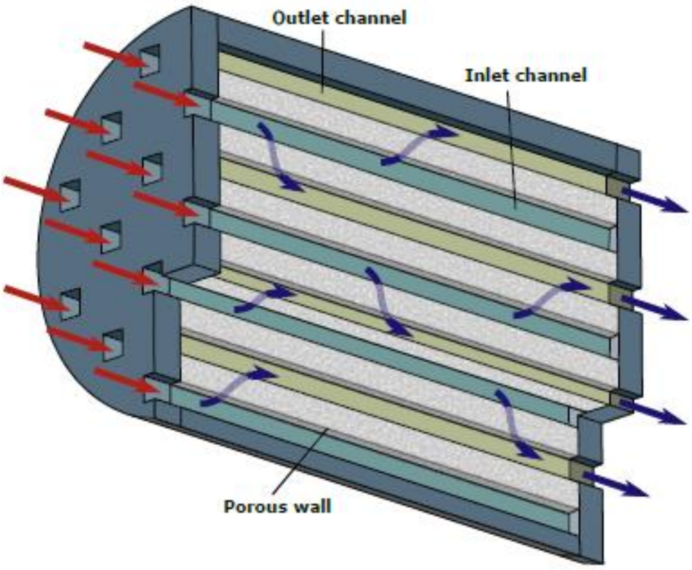

Figure 9: Cross section of a wall flow monolith.

A model of a gasoline particulate filter (GPF) has been developed using a single-channel approach. The underlying assumption of the single-channel approach is that the inlet condition, and hence behaviour, of all pairs of inlet and outlet channels in the device are identical. This mitigates the need to model more than one pair of channels. This is a common choice and is justified on the basis that it enables computationally efficient simulations without incurring a significant loss of precision [2].

The model has been developed and tested extensively in the context of diesel exhaust (for which there is a lot of data available in the scientific literature). The model includes the ability to describe the size-dependent filtration of exhaust particles. Full details of the model have been reported in the scientific literature [2]. Open access versions of the papers describing the model development are also available [3, 4].

3.1 Results

One of the key drawbacks of particulate filters is that they restrict the ease with which exhaust can flow through the exhaust system. This can be quantified in terms of the pressure drop that is observed across the filter. Understanding how the particles and the operation of the vehicle affect the pressure drop (and in particular, how quickly the pressure drop increases during operation) is an important aspect of designing a viable exhaust aftertreatment system.

The pressure drop can be calculated by the particulate filter model. Figure 10 shows the simulated versus experimental pressure drop through a GPF fitted to a multi-cylinder GDI test engine. Each point shown on the graph represents a steady-state operating point (there are 16 in total). The operating points span engine load and speed in the range 3—18 bar and 1500—4000 rpm. In this set of simulations, the pressure drop is purely a function of the structure of the filter and the rate of exhaust flow through it. No particles were included in the simulations.

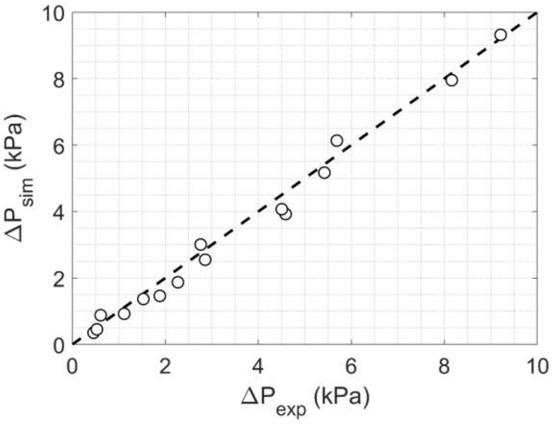

Figure 10: Simulated versus experimental pressure drop in a clean particulate filter.

Figure 11 and Figure 12 show the predicted pressure drop for cases where particles have been introduced in the simulations. The longer the loading time (i.e. the longer the time for which particles are allowed to accumulate), the higher the pressure drop. In each case, the permeability parameter in the model (which controls the ease with which exhaust can flow through the filter and hence the pressure drop) was adjusted to compensate for the additional pressure drop to restore agreement between the simulations and the experiments. The purpose of doing this was to understand the sensitivity of the pressure drop to the loading time in the experiments, and the consequent effect on the model parameters.

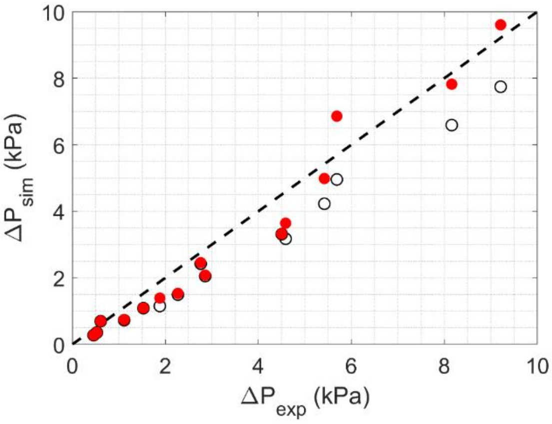

Figure 11: Simulated versus experimental pressure drop in a particulate filter after 20 minutes of loading. Red points consider the effect of the trapped particles. White points ignore the effect of the trapped particles.

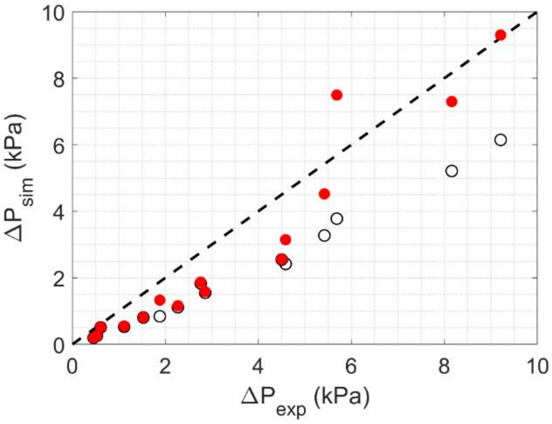

Figure 12: Simulated versus experimental pressure drop in a particulate filter after 40 minutes of loading. Red points consider the effect of the trapped particles. White points ignore the effect of the trapped particles.

4 Conclusion

The ultimate goal of developing mathematical models is to reduce the need for experimental measurements because experiments are time consuming and expensive to run. The models presented in this report are not at that stage yet because they still require additional experimental data to validate the models, and these experiments fall outside the scope of this project. The results in this report demonstrate the application of the models as complementary tools to experimental studies.

A model has been developed to simulate the evolution of particles and condensation of SOF in exhaust sampled from an engine as it passes through a dilution system into a particulate measurement device. A sensitivity analysis was performed to assess the effect of the sample dilution on the SOF fraction present when measuring the particles emitted from a single-cylinder GDI test engine.

A gasoline particulate filter (GPF) model that includes a size-dependent treatment of the filtration efficiency has been developed to support fundamental understanding of what happens to particulate emissions as they pass from the engine through the exhaust system to the tailpipe of a vehicle. The ability of the model to describe the pressure drop through a GPF is demonstrated against experimental data. A sensitivity analysis was performed to support the interpretation of experimental data from a multi-cylinder GDI test engine by investigating the impact of particle loading times on the observed pressure drop.

Overall, the models serve to support the design and interpretation of the experiments. It is much easier and cheaper to run a simulation compared to performing an experiment, potentially saving time and money.

5 Deviations from Annex 1

This deliverable includes results from extra calculations from CMCL, in addition to the calculations that were defined in the description of work. These extra calculations were possible thanks to the budget shift in 2018 that was approved by the project officer on November 14th 2018, and that is described in the Period 2 report under Deviations.

6 Bibliography

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Project partners:

#	Type	Partner	Partner Full Name
1	IND	HORIBA	Horiba Europe GmbH
2	IND	Bosch	Robert Bosch GmbH
3	IND/SME	CMCL	Computational Modelling Cambridge Limited
4	IND	TSI	TSI GmbH
5	HE	UCAM	The Chancellor, Masters and scholars of the University of Cambridge
6	HE	ULL	Université des Sciences et Technologies De Lille – Lille I
7	IND	IDIADA	Idiada Automotive Technologie SA
8	IND	HORJY	Horiba Jobin Yvon S.A.S.
9	IND/SME	UNR	Uniresearch BV

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Appendix A – Quality Assurance

The following questions should be answered by all reviewers (WP Leader, peer reviewer 1, peer reviewer 2 and the technical coordinator) as part of the Quality Assurance Procedure. Questions answered with NO should be motivated. The author will then make an updated version of the Deliverable. When all reviewers have answered all questions with YES, only then the Deliverable can be submitted to the EC.
NOTE: For public documents this Quality Assurance part will be removed before publication.

Question	WP Leader	Peer reviewer 1	Peer reviewer 2	Technical Coordinator
	Philipp Kreutziger	Amit Bhave	Jürgen Spielvogel	Marcus Rieker
1. Do you accept this deliverable as it is?	Yes	Yes	Yes	Yes
2. Is the deliverable completely ready? If not, please indicate and motivate required changes.	Yes	Yes	Yes	Yes
3. Does this deliverable correspond to the DoW?	Yes	Yes	Yes	Yes
4. Is the Deliverable in line with the PEMs4Nano objectives?	Yes	Yes	Yes	Yes
a. WP Objectives?	Yes	Yes	Yes	Yes
b. Task Objectives?	Yes	Yes	Yes	Yes
5. Is the technical quality sufficient?	Yes	Yes	Yes	Yes

Appendix B – Abbreviations / Nomenclature

Table B-1 List of Abbreviations / Nomenclature.

Symbol / Shortname	
EEPS	Engine Exhaust Particle Sizer
GDI	Gasoline direct injection
GPF	Gasoline particulate filter
ICE	Internal combustion engine
RPM	Revolutions Per Minute
SI	Spark ignition
SOF	Soluble organic fraction
SRM	Stochastic reactor model