



## **Publishable Executive Summary**

Within the PEMs4Nano project, in particular within WP3 "Measurement integration into systems development", the Model Guided Application (MGA) is aimed to progress beyond the state-of-the-art in simulating the formulation and evolution of particles in the context of GDI SI engine. The MGA combines the physico-chemical models with advanced statistical algorithms to simulate the particulate matter (PM) and particle number (PN) emissions on an internal combustion (IC) engine (single-cylinder and multi-cylinder) as well as a vehicular level. Typical particulate formation models for IC engines have focused on describing carbonaceous (soot) particles as they were the dominant particulate emission type in terms of mass and number. Novel exhaust after treatment (diesel particulate filters) and engine (gasoline direct injection) technologies have caused other, liquid-like, particulates to become increasingly important when considering PN emissions. The present particle formation models are not well-suited to modelling PM and PN emissions from modern vehicles, and the MGA in the first instance, addresses this technology gap. Within WP2 and WP3, a novel particulate formation model that includes a description of liquid-like particles has been formulated and implemented into the (Stochastic Reactor Model) SRM Engine Suite software. The coupled software is validated against measurements data from a single cylinder research engine at Bosch for in-cylinder pressure, gas phase emissions and particle phase emissions over a range of engine loads and speeds. Furthermore, the effect of the sampling system conditions on the evolution of the predicted engine-out particle size distributions and composition is investigated using chemical reactor networks. The validated MGA workflow comprising of the SRM Engine Suite and the reactor network is directly applicable to simulate the engine-out (and sampled) PSDs from single and multi-cylinder GDI SI engines. In this work, the MGA emphasizes the role that dilution plays in terms of the presence of soluble organic fractions and the influence on the resulting PSD, and highlights the need for further experimental composition analysis of sulphates  $(SO_x)$  within the engine-out particulates.



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