

Modeling of the Soot Oxidation in Gasoline Particulate Filters

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ABSTRACT

The share of gasoline engines based on direct injection (DI) technology is rapidly growing, to a large extent driven by their improved efficiency and potential to lower CO₂ emissions. One downside of these advanced engines are their significantly higher particulate emissions compared to engines based on port fuel injection technologies [1]. Gasoline particulate filters (GPF) are one potential technology path to address the EU6 particulate number regulation for vehicles powered by gasoline DI engines. For the robust design and operation of GPFs it is essential to understand the mechanisms of soot accumulation and oxidation under typical operating conditions.

In this paper we will first discuss the use of detailed numerical simulation to describe the soot oxidation in particulate filters under typical gasoline engine operating conditions. Laboratory experiments are used to establish a robust set of soot oxidation kinetics. The filter model and oxidation kinetics are validated using a large set of experimental data from laboratory reactor as well as vehicle experiments. With the validated model and parameters the impact of key operating parameters will be discussed, with special focus on passive soot oxidation mechanisms under normal vehicle operating conditions. Results show that short oxygen pulses during fuel cuts are the dominant passive regeneration mechanism. Results also provide insight into potential "worst case" conditions. Based on the insight from the detailed model a reduced 0D model is developed and described, which could be used for real time soot estimation.

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INTRODUCTION

The share of gasoline engines based on direct injection (DI) technology is rapidly growing, to a large extent driven by their improved efficiency and potential to lower CO₂ emissions. One downside of these advanced engines are their significantly higher particulate emissions compared to engines based on port fuel injection technologies [1]. Gasoline particulate filters (GPF) are one potential technology path to address the EU6 particulate number regulation for vehicles powered by gasoline DI engines. During vehicle operation the particulates are trapped in the GPF and accumulate over time. More than 90% of the emitted particulate mass is soot, consisting primarily of elemental carbon and small fractions of hydrocarbons like lubricant oil and fuel. The amount of soot in the filter can be reduced by oxidation at elevated temperatures and presence of an oxidant, e.g. oxygen, under release of heat.

With increasing soot load of the filter the resistance to flow increases, resulting in an increased backpressure. This can have negative impact on the performance of the engine as well as the fuel economy. Under certain operating conditions and high soot loads the heat release during oxidation can also result in significant thermo-mechanical stresses in the filter with a risk for failure of the component.

For a robust control during vehicle operation it is therefore required to enable continuous information about the soot loading state of the GPF. This requires knowledge about the accumulation rate as well as the rate of soot oxidation. Whereas significant experience exists for applications with diesel engines and diesel particulate filters, only limited knowledge is available for gasoline applications. Of special practical interest is a solid fundamental understanding of conditions, which enable a passive oxidation of the accumulated soot. In this context passive means that the oxidation occurs under normal operation of the engine, without any measures that would enhance its rate or generally facilitate it. While this is understood for diesel engines the dominant mechanisms do not apply to gasoline engines. Gasoline engines are typically operated stoichiometric; hence, under normal operating conditions no oxygen is available. In addition, the NO₂, which is very effective in diesel applications, is reduced to low levels over the upstream three-way catalyst and not available for the oxidation of soot.

With respect to component protection it is also of interest to determine which conditions represent so called worst case conditions, leading to extreme thermal stress within the filter. This knowledge is crucial for the development of strategies and controls to prevent them.

Combined with well-designed experiments, detailed mathematical models, considering the relevant physics within a particulate filter combined with models describing the chemical reactions of interest

are a powerful tool to develop the above mentioned fundamental understanding. They allow for easy access to detailed information even within the filter component and enable efficient parametric studies. A lot of literature exists describing such detailed filter models, respecting the conservation of mass, energy and momentum [11,12]. For most purposes one and two dimensional models are sufficient and allow for an efficient computational effort. Some of the models have been converted to validated and standardized software tools. One example used by a broad technical community is the software package AxiSuite [3], which is also used in our study.

Besides the application in fundamental studies, models are also powerful tools in engine controls. They can be used as virtual sensors in open and closed loop controls. Due to the limited onboard CPU capabilities and the need for real time operation, detailed models are typically computationally too expensive. Simpler, reduced models are required. The detailed models, however, can be used to develop such reduced models and, in addition to experimental data, help to calibrate them.

In this paper we first want to explore engine and vehicle operating conditions which facilitate a passive soot oxidation in a gasoline environment. Basis will be a detailed filter model, provided by the AxiSuite software package. Since the focus is the oxidation of soot, a key requirement is the availability of a suitable set of reaction kinetics. Examples from the validation of the detailed model and kinetics under real world driving conditions will be provided. The effect of a range of exhaust parameters will be discussed. In the second part of the paper a reduced model for potential application in a vehicle control system will be described. The reduced model is parameterized with the help of the validated detailed model.

MODELING

In this contribution two types of component models will be used and discussed: A detailed 1D filter model and a reduced 0D filter model, which has the potential to be used in control algorithms. Common to both component models are (a) the kinetics used to describe the rate of oxidation of soot and (b) a simple, map based engine model providing the information about the transient particulate emissions of the engine.

Filter Model

Detailed Model

In our work the AxiTrap tool available in the AxiSuite software package was used as detailed filter model. The filter model considers for the conservation of mass, energy and momentum. Details about the implemented physics and numerical methods are provided in [3]. The simulations were in most cases limited to a one dimensional treatment of the filter, considering only changes along the main flow axis (z) and assuming uniform distribution of flow, concentrations and temperature in radial direction. To describe the characteristics of the filter materials used the corresponding physical properties were provided. Catalytic reactions of the TWC coating, if present, are considered using a standard set of rate expressions. Details about the description of the oxidation reaction of soot will be discussed below.

Reduced Model

An effective approach to obtain a reduced, computationally less expensive model is to reduce it to a quasi-homogeneous, 0-dimensional description of the filter [5]. Although not capable of exactly describing all the phenomena occurring in a particulate filter it is well suited to capture the general phenomena and, since it is physics based, allows for relatively easy and flexible parameterization. The model uses a single energy balance, eqn. (1), lumping the gas and solid phase together.

$$\frac{dT}{dt} = \frac{(-\Delta H_R) \cdot R_{C+O_2}}{V_{GPF} \cdot \rho_{GPF} \cdot c_{ps}} - \frac{\dot{m}_G \cdot c_{pG} \cdot (T - T_{in})}{V_{GPF} \cdot \rho_{GPF} \cdot c_{ps}} \quad (1)$$

In this equation T represents the temperature, t the time, ΔH_R the reaction enthalpy, R the reaction rate, $\dot{m}$ the gas mass flow rate and c_{pG} and c_{ps} the specific heat capacity of the gas and solid phase, respectively. The filter volume and density are described by V_{GPF} and ρ_{GPF} .

The conservation of the mass of soot and oxygen within the filter is also considered assuming uniform deposition and concentrations within the component, eqn. (2) and (3).

$$\frac{dm_c}{dt} = \dot{m}_G \cdot \eta_f \cdot w_{C,in} - M_C \cdot v_C \cdot R_{C+O_2} \quad (2)$$

$$\frac{dw_{O_2}}{dt} = \frac{\dot{m}_G \cdot (w_{O_2,in} - w_{O_2}) - M_{O_2} \cdot v_{O_2} \cdot R_{C+O_2}}{V_{GPF} \cdot (1 - \varepsilon_{GPF}) \cdot \rho_G} \quad (3)$$

Here m represents the mass, w the mass fraction, η the filtration or collection efficiency, M the molecular weight and ε the porosity of the filter.

For the dynamic simulation transient information is required as boundary condition for the mass flow, the inlet temperature, the oxygen concentration and the particulate raw emissions. Standard sensors are available for the first three variables, enabling their simple and cost effective measurement on a vehicle. For the particulate emissions no reliable standard sensor is available to date. Excellent progress has been made in the development of particle mass and number measuring PEMS equipment [9]. Such equipment, however, is limited for use in dedicated experiments and not for regular onboard measurement. Therefore, virtual soot sensors based on models are required for the above simplified filter model. The approach chosen in this work will be described below.

For the application the reduced model has been implemented in Matlab/Simulink. The generic structure of the Simulink model is shown in Figure 1.

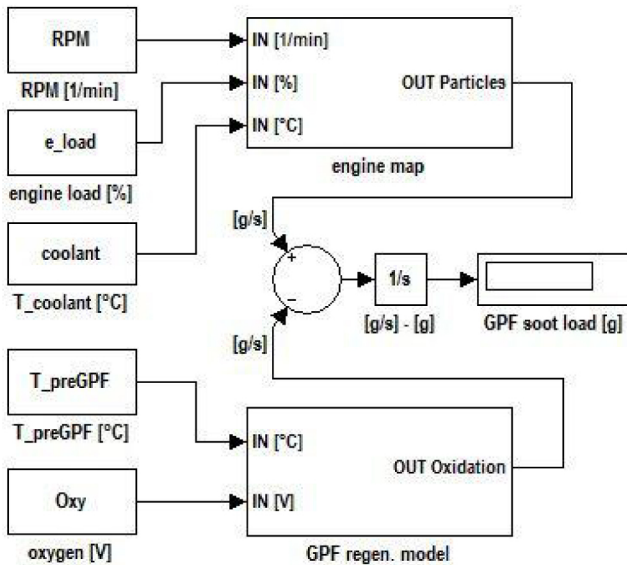


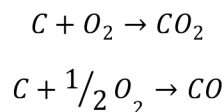
Figure 1. Schematic of simplified filter model

The model is separated into sub-models describing the rate at which particulates are emitted from the engine, the “engine emissions” module, and sub-models describing the rate at which soot is oxidized. The advantage of a 0D Simulink model versus complex simulations is the visualization of the required data and the relatively easy transfer to a vehicle infrastructure. Using feed forward maps, rather than complex algorithms, allows the adaption and calibration to measured data. As one can see from Fig. 1 does the model require only 5 input variables that are already available in most gasoline powered vehicles, either from hardware sensor or virtual sensors like catalyst temperature models.

Soot Oxidation Kinetics

Common to both models, the detailed AxiSuite based model as well as the simplified 0D model, is the need for reliable soot oxidation kinetics. Soot can be oxidized by a number of potential oxidants. In engine exhaust, O_2 and NO_2 are the most relevant oxidants. For gasoline applications with a modern TWC upstream of the filter the availability of NO_2 is further limited. Therefore, our current work has been focused and limited to oxygen.

In general, the oxidation of soot with oxygen follows one of the two following reactions paths:



The soot is either totally oxidized to CO_2 or only partially to CO. The distribution between both reactions is determined by the temperature and the availability of oxygen. Typically, a simple global reaction kinetic as provided by eqn. (4) is used to describe the soot oxidation [10,11]:

$$-\frac{dm_c}{dt} = A \cdot \exp\left(-\frac{E_a}{RT}\right) \cdot m_c^n \cdot p_{O_2}^r \quad (4)$$

Here E_a is the activation energy for the reaction and n and r are the reaction order in soot (carbon) and oxygen, respectively.

Since the generation of reasonably high quantities of GDI soot on vehicle has been challenging it was decided to perform the experimental work in this study using Printex U as a model soot. Printex U was found to be reasonably representative of GDI soot [2] and represents soot with fairly low reactivity due to its very high elemental carbon content. To obtain reliable oxidation kinetics laboratory experiments have been performed using thermo-gravimetric analysis (TGA). Details about the experimental method are provided in [2]. Focus was on temperatures below 550°C , a range for which limited data were available from past work for diesel applications. Results from isothermal measurements at temperatures between 300°C and 500°C in air are shown in Figure 2.

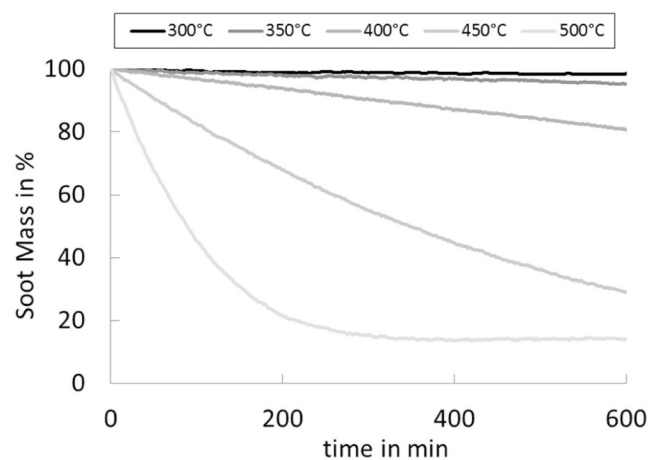


Figure 2. Experimental data from isothermal TGA measurements with Printex U model soot in air.

From the experimental data the reaction rates were extracted, providing for the pre-exponential factor as well as the activation energy. These data are shown in Figure 3. With respect to the reaction order values of 1 were found to fit for oxygen and soot.

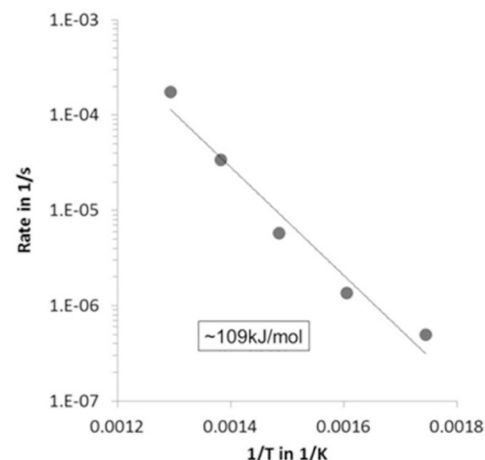


Figure 3. Reaction rates for soot oxidation in air from isothermal TGA.