

Modeling of heavy duty diesel soot filter regeneration by calibrating with engine-specific soot reactivity

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Background / Objectives

Simulation has become an important tool for the design of exhaust systems. One of the many desired applications of these models is to predict soot regeneration at various conditions. The challenge is that soot reactivity varies with fuel type [1,2], from one engine to another or at different points of an engine map [3,4]. Many studies have shown differences in soot reactivity depending on their morphology, nanostructure [1,3] and composition [4]. For example, Figure 1a shows that 6 soot samples collected on different engines and/or different modes show a different response to oxidation in air. The objective of this work was to develop a methodology for creating accurate soot models for various soot samples but with minimal characterization.

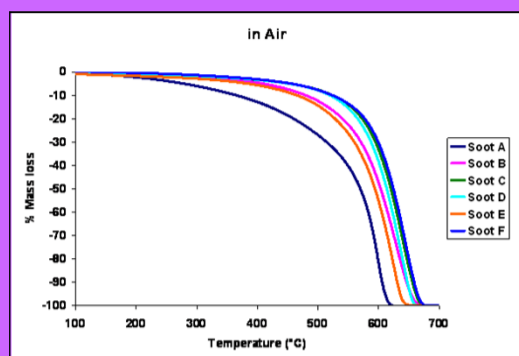


Figure 1a: Soot mass loss as a function of temperature for 6 soot samples collected on different engines and/or different modes.

[1] K. Al-Qurashi et al., "Impact of exhaust gas recirculation (EGR) on the oxidative reactivity of diesel engine soot", Combustion and Flame, 155, 675-695 (2008).
 [2] Juhun Song et al., "Impact of alternative fuels on soot properties and DPF regeneration", Combust. Sci. and Tech., 179, 1991-2037 (2007).
 [3] R. Vander Wal et al., "HRTEM study of diesel soot collected from diesel particulate filters", Carbon, 45, 70-77 (2007).
 [4] J. Rodriguez-Fernandez et al., "Characterization of the diesel soot oxidation process through optimized thermogravimetric method", Energy and Fuels, 25, 2039-2048 (2011).

Methodology

The reactivity of soot with O₂ and NO₂ can depend on many parameters such as morphology, composition and surface species. Predicting soot reactivity from this information is a very difficult challenge that would require in depth characterization of all soot samples.

To be able to create models with minimal characterization, reactors and Thermo-Gravimetric Analysis (TGA) were used to directly access to oxidation kinetics in O₂-rich and NO₂-rich environments.

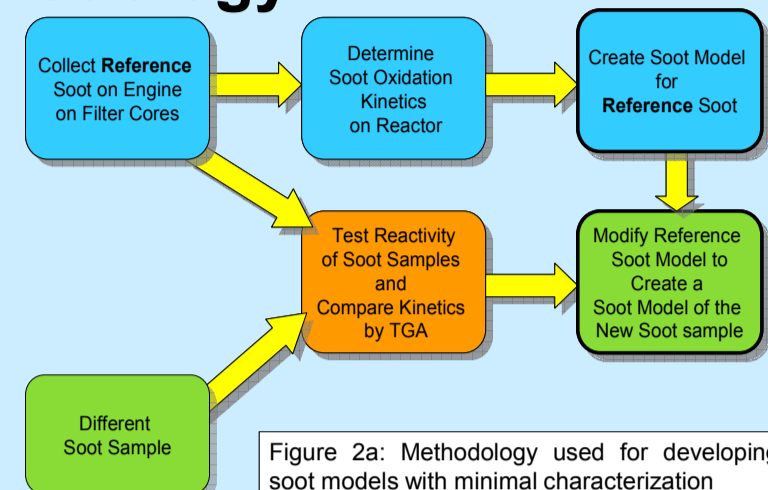


Figure 2a: Methodology used for developing soot models with minimal characterization

As described by Figure 2a, to create a robust initial model, a "reference" soot sample was collected on filter cores in an engine exhaust. The oxidation kinetics were measured on reactor and a model was developed from these data. Then, the "reference" and a "new soot" sample collected on a different engine were tested by TGA in similar conditions to compare oxidation rates by NO₂ and O₂. Finally, the relative difference in oxidation kinetic parameters measured by TGA was used to modify the "reference" soot model to create a model for the "new soot".

Reactor Study of Soot Reactivity

- One soot sample collected directly on non-coated filter cores in the exhaust of an engine was used as a reference for this study (Figure 3a). The core holder was positioned downstream of a DOC to better represent reality by partially oxidizing the SOF (Soluble Organic Fraction) part of the soot.
- The filter cores, loaded with soot, were then studied on a reactor where CO, CO₂, NO and NO₂ were measured with an FTIR downstream of the core to measure Carbon consumption and reaction kinetics.
- During the test, effects of temperature, NO₂ and O₂ concentrations were studied. Figure 3b represents a gas concentration profile used during this study.
- The reactor results were used to fit the kinetic parameters for each reaction considered in the model (see below). Figure 3c and 3d respectively show a comparison of the model to the measured data as a function of time and as a parity plot.

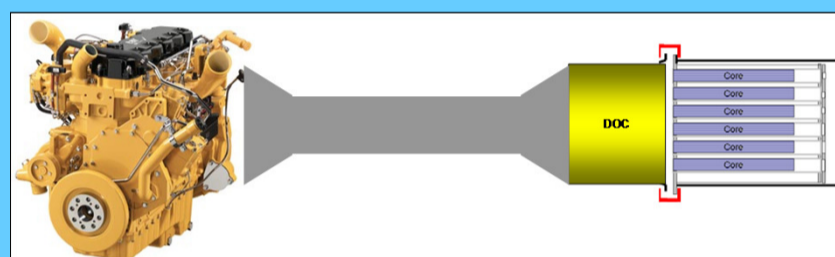


Figure 3a: Soot samples are directly collected in the engine exhaust, on uncoated filter cores, downstream of a DOC.

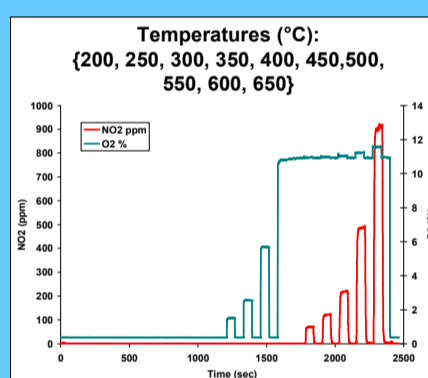


Figure 3b: Gas concentration profile for reactor study

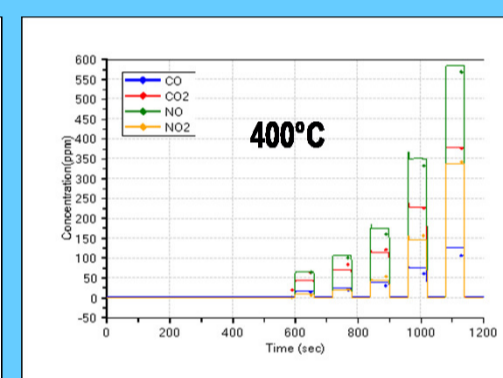


Figure 3c: Comparison between measured data (dots) and fitted model (lines).

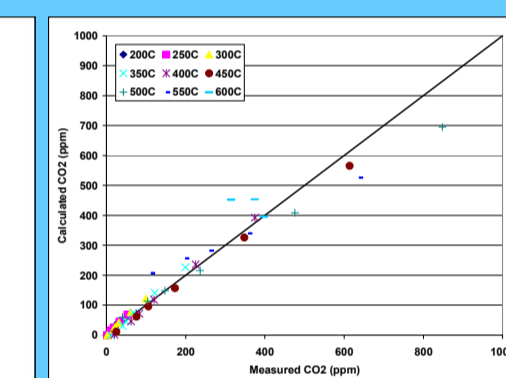
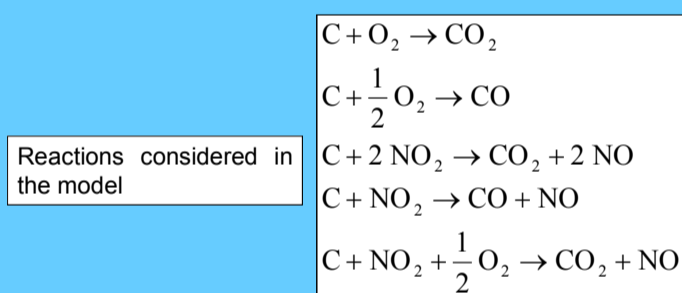


Figure 3d: Parity Plot for CO2 concentration



Thermo-Gravimetric Comparison of Different Soot Samples

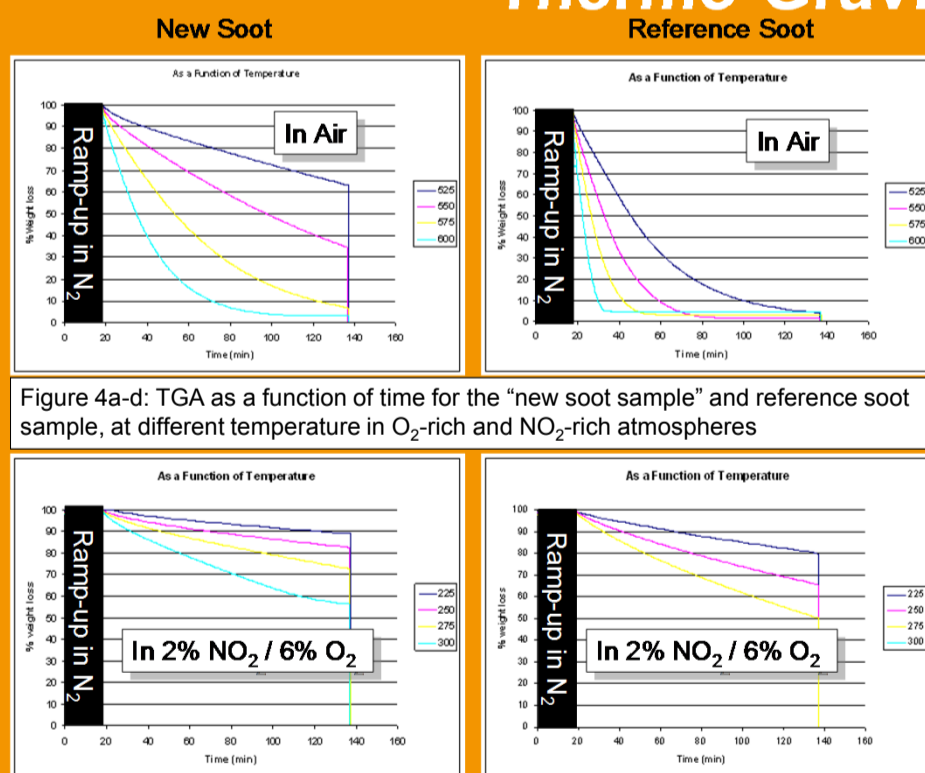


Figure 4a-d: TGA as a function of time for the "new soot sample" and reference soot sample, at different temperature in O₂-rich and NO₂-rich atmospheres

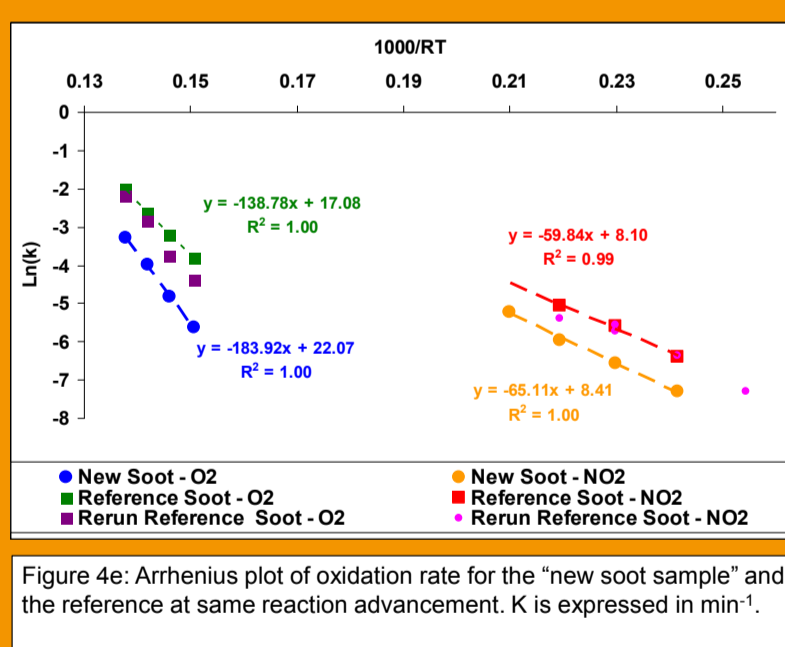


Figure 4e: Arrhenius plot of oxidation rate for the "new soot sample" and the reference at same reaction advancement. K is expressed in min⁻¹.

Now that a soot model is available for the reference soot, TGA can be used to compare reactivity between a "new soot" sample and the reference. The comparison was done at temperatures between 525°C and 600°C in air and between 225°C and 300°C in 2% NO₂ / 6% O₂ atmosphere.

Directly from the mass loss as a function of time presented in Figures 4a-d, the lower reactivity of the "new soot" relative to the reference can be observed. The oxidation rates are measured at a similar conversion for both soot samples and compared on an Arrhenius plot (Figure 4e). The activation energies for oxidation by O₂ and by NO₂ are in agreement with the different values reported in literature with respectively, 140-180 kJ/mol and 60-65 kJ/mol. The difference in reactivity between soot samples is mostly due to differences in the pre-exponential coefficients.

This relative difference in pre-exponential coefficients is the information used to modify the reference soot model and create a model for the "new soot".

Engine Data and Modeling

Data on soot passive regeneration generated on the engine that produced the reference soot sample was used to check the reference model created from the reactor data. A non-coated and a coated filter were loaded with soot in the same conditions. Then, the engine was run at C50 or C100. The filter was periodically removed from the system to measure its mass variation as a function of time. Figure 5a shows a good agreement between the measured soot loading (dots) compared to the model prediction (lines). NO₂ at filter-out was also measured during the test. The model was also capturing correctly the NO₂ variations with soot loading (not showed here).

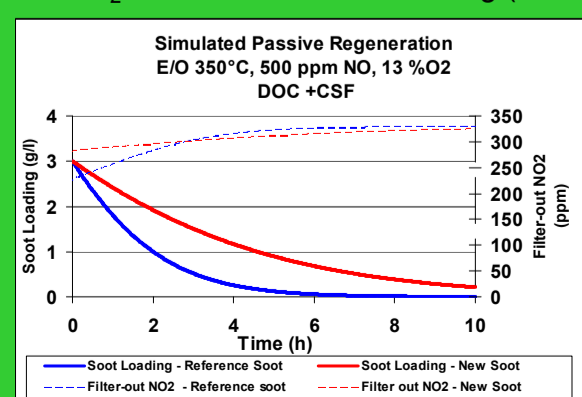


Figure 5b: Simulated passive regeneration with models of reference and "New" soot sample.

The different soot models (reference created from reactor data and "new Soot" model created from relative reactivity differences measured on the TGA) can be used to simulate soot regeneration for various engine conditions. An example is given in Figure 5b.

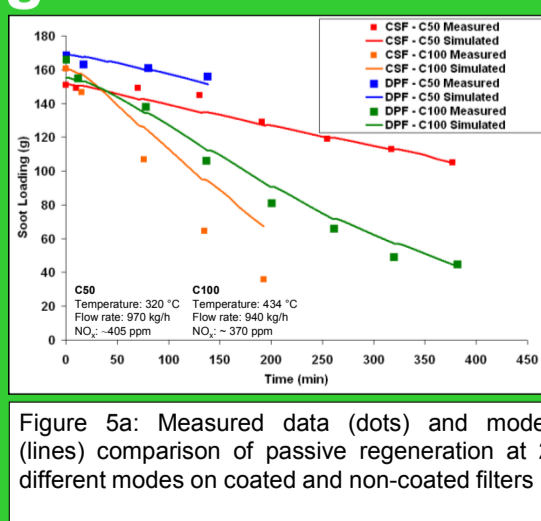


Figure 5a: Measured data (dots) and model (lines) comparison of passive regeneration at 2 different modes on coated and non-coated filters

Conclusions / Path Forward

A methodology to simulate soot from different origins was presented. First, a reference soot sample was collected on engine and tested at various conditions on reactor. From these data, a model was created and verified against engine data.

The second step of this methodology was to use a different soot sample from another origin (different engine) and compare its reactivity to the reference soot sample by solely using thermo-gravimetric analysis. The relative difference of reactivity was used to create a model of this "new soot" sample.

The path forward of this study is to validate the "new soot" model with engine data.