Chemical Engineering Science 137 (2015) 69–78

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Modeling and simulation of soot combustion dynamics in a catalytic diesel particulate filter

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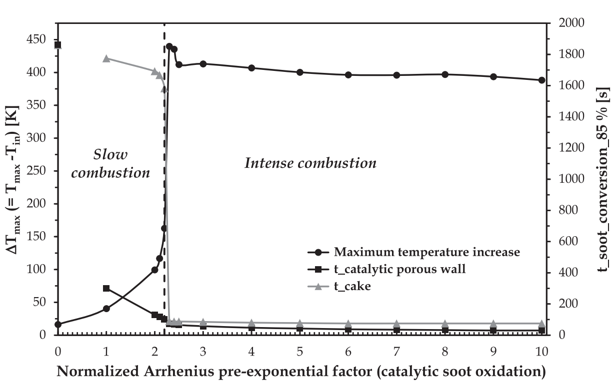
HIGHLIGHTS

- A CFD-based model of soot regeneration developed for a catalytic diesel particulate filter.
- Effect of the catalyst activity on the filter regeneration dynamics simulated.
- Transition from slow (uniform combustion) to fast (front propagation) regeneration with increasing catalyst activity.
- The highest temperature rise when soot in the catalytic porous wall of the filter and cake burn together.
- Time for filter regeneration insensitive to the increase in catalyst activity beyond a threshold level.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 20 February 2015
Received in revised form
5 June 2015
Accepted 6 June 2015
Available online

Keywords:
Computational fluid dynamics
Catalytic diesel particulate filter
Soot combustion
Regimes of regeneration
Catalyst activity
Catalytic pilot

ABSTRACT

In the work presented in this paper, a two-dimensional mathematical model of soot regeneration was developed for a single-channel catalytic diesel particulate filter. The commercial computational fluid dynamics (CFD) code ANSYS Fluent 15.0 was used to simulate the gas flow field, whereas the regeneration kinetics was implemented through user-defined-subroutines. Both mechanisms of catalyzed and non-catalyzed (i.e., thermal) oxidation were used to describe combustion of the soot trapped inside the porous wall of the filter. Conversely, only non-catalyzed oxidation was assumed for the cake layer. The aim of the work was at investigating the effect of the catalyst activity on the regeneration dynamics of the filter in the light of the thermal interaction between combustion of the soot in the (catalytic) porous wall and combustion of the cake. To this end, computations were run by increasing the pre-exponential factor in the Arrhenius equation for the catalytic reaction rate, thus simulating the effect of increasing catalyst activity.

Numerical results have shown that, as the catalyst activity is increased, a transition occurs from a regime of slow combustion, in which regeneration proceeds in a substantially uniform manner over the filter, to a regime of intense combustion, in which regeneration proceeds by a reaction front moving upstream and downstream. The regime of slow combustion is characterized by low temperature rise (difference between the maximum filter temperature, T_{max}, and the inlet gas temperature, T_{in}, lower than 100 K) and long time for cake consumption and, thus, filter regeneration (~1800 s). It is established when the catalyst activity is too low to appreciably affect combustion of the cake. Thus, combustion of the cake occurs independently of what happens in the porous wall of the filter. In contrast, the regime of

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http://dx.doi.org/10.1016/j.ces.2015.06.011

intense combustion is characterized by high temperature rise – $(T_{max}-T_{in})$~400 K – and short time for regeneration (~100 s). It is established when the catalyst activity is high enough to make the porous wall of the filter an effective pilot for the cake. For this regime, the highest temperature rise is found under conditions that maximize the synchronization between combustion of the soot in the porous wall of the filter and combustion of the cake. When such a synchronization is attained, the time for filter regeneration becomes substantially insensitive to variations in the catalyst activity.

1. Introduction

Diesel particulate filters (DPFs) are the most effective option for removing particulate matter (PM) from diesel engine exhaust (Johnson, 2009). A DPF is generally made of ceramic materials, such as cordierite or silicon carbide. It consists of thousands of square parallel channels, with the opposite ends of adjacent channels being plugged. The exhaust gas enters the inlet channels and passes through the porous walls to adjacent outlet channels. This path allows PM, which is mostly made of carbonaceous particles called soot, to be retained in the inlet channels (Bensaid et al., 2009a, 2009b). More specifically, the soot particles are first trapped inside the porous walls of the filter. When the maximum packing density is reached, the walls become substantially impermeable to the particles, and a soot layer, also called cake, is built up onto the porous filter surface. The existence of a cake layer is an important advantage for the filtration performance. Indeed, the cake itself acts as a filter and most of the soot is trapped under this form.

The collected soot increases the backpressure of the diesel engine reducing its efficiency. Thus, the DPF needs to be periodically regenerated (cleaned) by soot combustion (Fino and Specchia, 2008; Warner et al., 2010). Unfortunately, the temperature of the diesel exhaust gas is too low (200–500 °C) to initiate and maintain soot oxidation. To raise the exhaust gas temperature up to the point that soot oxidation can be self-sustained in the filter at fast enough rates (>600 °C), external or engine (i.e., active) means (e.g., fuel burners, electric or microwave heating, injection of fuel in the exhaust, recirculation of exhaust gas, etc.) can be employed. Such an approach, also referred to as thermal regeneration, incurs additional energy costs and requires complex means of control. Furthermore, in some cases, it can lead to local temperature excursions sufficiently high to damage the DPF (Belloir et al., 2007; Koltsakis et al., 2007). Alternatively or complementarily, catalytic measures can be used to achieve soot oxidation at lower temperatures (250–550 °C) and/or to shorten the regeneration time period, thus allowing for energy saving (at an added cost of the catalyst).

Fuel borne catalysts (FBCs), i.e., additives that are mixed with the fuel to lead to the formation of catalyst-doped soot during combustion in the engine, have been widely used as catalytic regeneration system (Stratakis and Stamatelos, 2003; Rocher et al., 2011). The FBC approach inherently requires a continuous additive supply in the fuel. Furthermore, the additive consumption leads to the accumulation of metal oxide "ash" inside the DPF. These problems can be overcome by attaching the catalyst directly onto the DPF.

Extensive research efforts have been focused on catalytic (catalyst impregnated or coated) DPFs (CDPFs). However, there is still no general consensus regarding their ability to oxidize soot at low temperatures and under conditions relevant to practical applications (Southward et al., 2010).

The regeneration performance of a CDPF is strictly dependent on the catalyst activity which, in turn, is strongly affected by the efficiency of the contact between the soot particles and the active sites of the catalyst particles (Kumar et al., 2012; Bensaid et al., 2013). In CDPFs, the soot/catalyst contact is especially difficult for the cake layer, which is accumulated (and somewhat segregated) on top of the catalytic wall of the filter (under such conditions, the surface area available for the interaction between the two solid phases is very low). Conversely, the soot trapped inside the catalytic wall of the filter can more easily come into contact with the catalyst.

Owing to the poor cake/catalyst contact, CDPFs allow a much lower decrease in the regeneration temperature (10–40 °C) than that attained with FBCs (140–250 °C) (Hinot et al., 2007). Furthermore, sharp temperature fronts have also been observed during regeneration of CDPFs. This issue has been profusely investigated by Professor Luss' group by means of infrared measurements of the spatiotemporal temperature rise (see, e.g., Chen et al., 2009, 2010, 2011a, 2011b; Martirosyan et al., 2010). From these results, it can be argued that, in a CDPF, the interaction between the catalyst and the cake is mainly thermal (rather than chemical) in nature: the soot in contact with the catalyst (i.e., the soot trapped inside the catalytic wall of the filter) first ignites, thus generating the heat that allows to initiate and sustain the combustion process of the cake. In other words, the catalyst acts as a pilot for the cake, whose regeneration remains essentially thermal.

On the other hand, the regeneration dynamics of the cake is also affected by the distribution of the gas flow inside the filter (Bensaid et al., 2010). Such a distribution is not easily predictable and, at the moment, it is still unclear how the contact between the gas and solid phases impacts on ignition and combustion of the retained soot.

The present paper fits in this framework with the aim at gaining insight into the effect of the catalyst activity on the regeneration dynamics of CDPFs in the light of the thermal interaction between combustion of the soot in the (catalytic) porous wall of the filter and combustion of the cake. To this end, a two-dimensional mathematical model of soot regeneration was developed for a single-channel CDPF. The commercial computational fluid dynamics (CFD) code ANSYS Fluent 15.0 was used to simulate the gas flow field, whereas the regeneration kinetics was implemented through user-defined-subroutines. Both mechanisms of catalyzed and non-catalyzed (i.e., thermal) oxidation were used to describe combustion of the soot trapped inside the porous wall of the filter. Conversely, only non-catalyzed oxidation was assumed for the cake layer. The regeneration dynamics of the filter was simulated, taking into account the coupling with the spatial distribution of the gas flow, for different values of the pre-exponential factor in the Arrhenius equation for the catalytic reaction rate, thus exploring the effect of varying catalyst activity.

2. Mathematical model

A CFD-based model of soot regeneration was developed for a single-channel catalytic DPF. Fig. 1 shows a schematic of the two-dimensional computational domain consisting of inlet channel, outlet channel and porous regions (wall of the filter and cake layer).