A CFD-BASED SIMULATION STUDY OF THE REGENERATION DYNAMICS OF A CATALYTIC DIESEL PARTICULATE FILTER

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Abstract
Transient CFD-based simulations of soot combustion in a single-channel catalytic diesel particulate filter were run to investigate the combined effects of inlet gas velocity and catalyst activity on the dynamics of regeneration.
Numerical results have shown that, at high inlet velocity, fast regeneration occurs at high catalyst activity, leading to high temperatures over the whole filter. Conversely, at low inlet velocity, fast regeneration occurs also at low catalyst activity. Furthermore, regardless of the catalyst activity, high temperatures develop only during the final stage of combustion of the residual cake accumulated close to the exit section of the filter, and remain limited to this zone. Thus, strategies able to prevent or mitigate such a *burn-up* phenomenon would be useful to allow fast regeneration under controlled temperature conditions.

Introduction
Experiments of regeneration of catalytic diesel particulate filters (DPFs) have shown that the soot accumulated as cake layer on top of the catalytic walls always burns via thermal path, being substantially segregated from the catalyst [1]. This explains why the formation of hot zones is a critical issue not only for thermal regeneration of DPFs, but also for regeneration of catalytic DPFs.
Combustion dynamics of the cake accumulated on planar catalytic single layer DPFs has been deeply investigated by means of infrared measurements of the spatiotemporal temperature (see, e.g., Refs. [2-6]). A transition has been observed from a regime of uniform combustion, characterized by slow regeneration and moderate temperature rise, to a regime of reaction front propagation, characterized by fast regeneration and high temperature rise, with increasing soot loading [2,6], oxygen concentration [2] and exhaust gas temperature [4]. This transition is accompanied by a decrease in the number of ignition points [6]. Indeed, in the case of slow regeneration, many ignition points coalescence with each other so that combustion occurs all over the surface. Conversely, in the case of fast regeneration, moving hot zones emanate from a few (distinct) ignition points, the number and locations of which are strictly dependent on the operating conditions. In particular,

as the inlet velocity is decreased, the location of single-point ignition shifts from downstream to upstream [2].

Recently, we developed a two-dimensional CFD-based model of soot combustion in a single-channel catalytic DPF [7]. Numerical results have shown that an abrupt transition from slow regeneration to fast regeneration may occur due to increased catalyst activity. In particular, under the simulated conditions of fast regeneration, the maximum temperature is attained when the catalytic wall is almost completely regenerated and, thus, the residual cake burns substantially alone. From these results, it has been concluded that, in order to prevent the formation of hot zones in catalytic DPFs, (thermal) combustion of the cake has to be driven by (catalytic) combustion of the soot trapped inside the filter wall.

The aim of the work presented in this paper was at identifying operating conditions under which the catalytic wall of the filter is able to sustain combustion of the cake in a uniform and gradual manner, thus allowing to get reasonably fast regeneration under controlled temperature conditions. To this end, simulations of filter regeneration were run with the previously developed model [7] by varying the catalyst activity at different inlet gas velocities. From numerical results, the operating map of the filter was built in the plane maximum temperature versus time of regeneration. The effect of the coupling between combustion of the soot in the catalytic wall and combustion of the cake on the spatiotemporal evolution of the filter temperature was investigated also in terms of ignition location of the cake.

Mathematical Model

The model is described in detail in Ref. [7]. It was developed by using the platform of the CFD code ANSYS Fluent 15.0 and, in particular, the porous medium model [9]. Figure 1 shows a schematic of the two-dimensional computational domain.

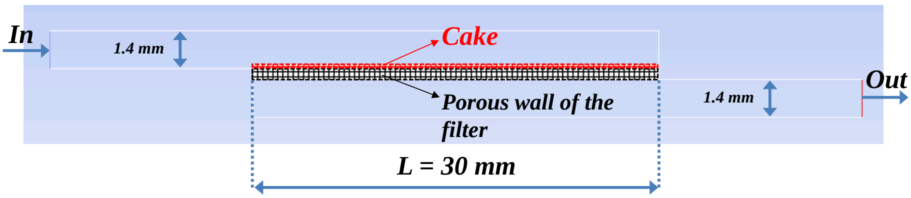

Figure 1. Schematic of the two-dimensional computational domain (not to scale) (thickness of the porous wall of the filter = 0.38 mm; initial thickness of the cake layer = 0.12 mm).

The kinetics of catalytic oxidation of diesel soot with oxygen proposed by Darcy et al. [8] was adopted. The soot oxidation rate is expressed as the sum of two contributions, a first contribution associated with “slow oxidation”, which involves all the soot present in the system, and a second contribution associated with “fast oxidation”, which involves only the soot directly in contact with the catalyst (0.4 % $Pt/CeZrO_2$). In the porous wall of the filter, both contributions of slow and fast oxidation were implemented. Furthermore, all the soot present was assumed to be in contact with the catalyst. In the light of the experimental results reported in Ref.

[1], the cake-catalyst contact was fully neglected. Thus, in the cake, only the slow contribution was implemented.

Simulations were run by varying the catalyst activity, i.e., the pre-exponential factor in the kinetic expression of "fast oxidation", at both low and high inlet gas velocity (V_{in} = 1 and 5 m/s). In particular, the ratio, *k*, between the pre-exponential factor used in the computations and the pre-exponential factor of the kinetics by Darcy et al. [8] was increased from 0 (thermal regeneration) to 10. The simulation (inlet and initial) conditions are listed in Table 1. All details about the numerical solution can be found in Ref. [7].

Table 1. Simulation conditions.

Inlet conditions	**Velocity** [m/s]	1; 5
	O_2 concentration [% mol]	15
	Temperature [K]	813
Initial conditions	**Velocity** [m/s]	0
	O_2 concentration [% mol]	15
	Soot concentration [kg/m^3]	15 (wall of the filter); 200 (cake)
	Temperature [K]	523

Results and Discussion

Figure 2 provides a general overview of the results obtained from simulations run by varying the catalyst activity (i.e., *k*) at different inlet velocities. The results at V_{in} = 3 m/s are from Ref. [7]. In particular, the figure shows the operating map of the filter in the plane maximum temperature attained during the regeneration process, T_{max}, versus time of regeneration, i.e., time of cake consumption, t_{cake}.

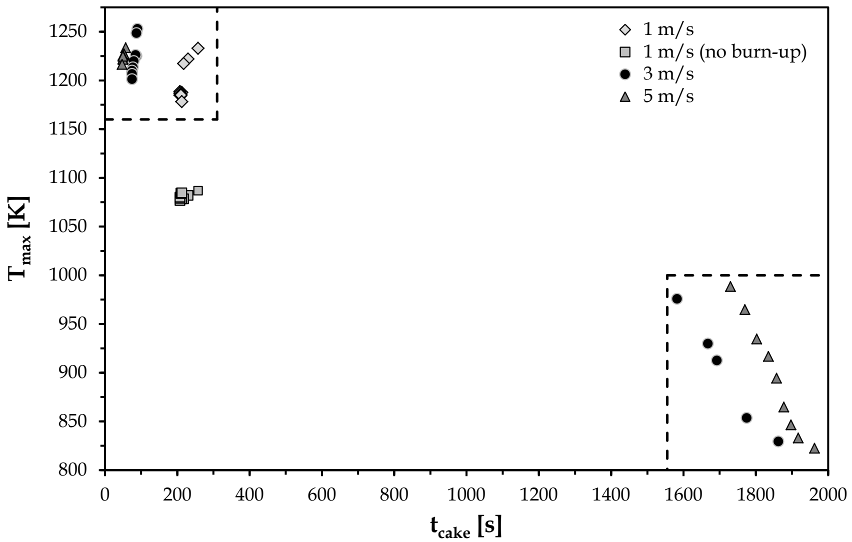

Figure 2. Operating map of the filter as built in the plane T_{max} versus t_{cake}.

All points fall within two zones of the plane (bounded by dashed lines): a first zone of low temperature and long time of regeneration or, alternatively, a second zone of high temperature and short time of regeneration. The first zone corresponds to a regime of slow regeneration characterized by substantially uniform combustion all over the filter. Conversely, the second zone corresponds to a regime of fast regeneration characterized by a reaction front moving along the filter. The regime of slow regeneration is not found at $V_{in} = 1$ m/s, whereas the regime of fast regeneration is found at all the values of velocity investigated.
From an applicative point of view, the short time of filter regeneration makes the regime of fast regeneration much more interesting than the regime of slow regeneration. Unfortunately, high temperatures characterize this regime.
In order to investigate the opportunity for reducing the temperature rise, while keeping short times of regeneration, the attention is here focused on the regime of fast regeneration at high velocity ($V_{in} = 5$ m/s) and low velocity ($V_{in} = 1$ m/s).
At $V_{in} = 5$ m/s, the regime of fast regeneration is established at high catalyst activity (i.e., $k > 5.1$). Under such conditions, combustion of the cake takes place according to a partially catalyst-assisted regeneration mode: catalytic combustion of the soot in the porous wall of the filter just provides local violent ignition for the cake, which thus burns substantially alone. Figure 3 shows the spatiotemporal evolution of the temperature of the filter wall at $k = 10$.

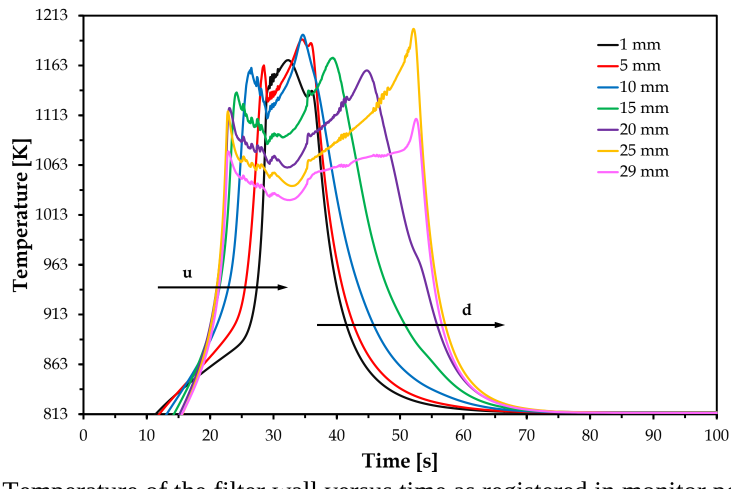

Figure 3. Temperature of the filter wall versus time as registered in monitor points located at different axial positions: $V_{in} = 5$ m/s; $k = 10$.

All the temperature time histories exhibit two dominant peaks. The first peak is associated with a reaction front propagating from downstream to upstream (u wave). Conversely, the second peak is associated with a reaction front propagating from upstream to downstream (d wave). During both the phases of propagation, high temperatures develop involving the whole filter. The same behavior has also

been found at V_{in} = 3 m/s [7].
At V_{in} = 1 m/s, the picture looks quite different as shown by the spatiotemporal evolution of the filter temperature in Figures 4 (low catalyst activity, k = 1) and 5 (high catalyst activity, k = 10).

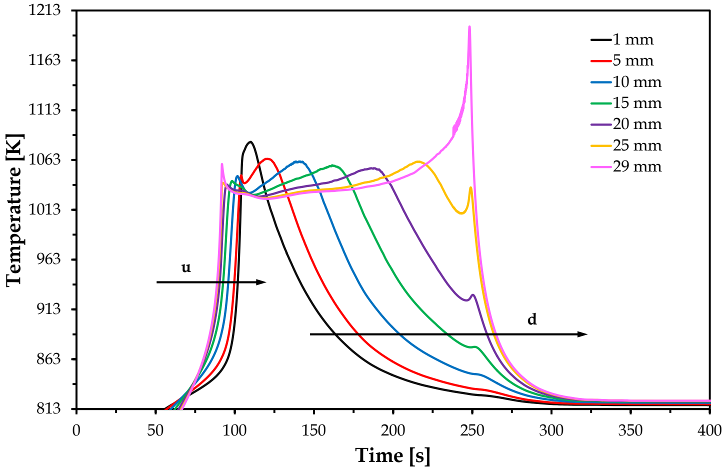

Figure 4. Temperature of the filter wall versus time as registered in monitor points located at different axial positions: V_{in} = 1 m/s; k = 1.

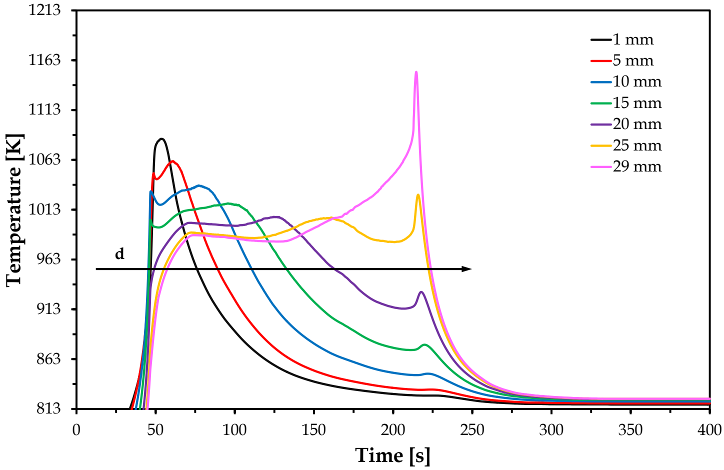

Figure 5. Temperature of the filter wall versus time as registered in monitor points located at different axial positions: V_{in} = 1 m/s; k = 10.

Differently from the high velocity case, at low velocity, regardless of the catalyst activity, combustion of the soot in the catalytic wall and combustion of the cake are synchronized with each other. Thus, a fully catalyst-assisted regeneration mode is established which allows a more uniform combustion of the cake. Indeed, most of the regeneration process takes place at low temperatures, whereas high

temperatures develop only during the final stage of combustion of the residual cake accumulated close to the exit section of the filter, and remain limited to this zone. Thus, strategies able to prevent or mitigate such a *burn-up* phenomenon would be useful to allow fast regeneration under controlled temperature conditions. This concept is better highlighted by the square symbols in Figure 2, which correspond to the results obtained at $V_{in} = 1$ m/s, when ideally stopping the regeneration process before the *burn-up* phenomenon can occur.
It is worth noting that, at $V_{in} = 1$ m/s, the increase in catalyst activity allows the ignition location of the cake to move from downstream to upstream (conversely, at $V_{in} = 3$ m/s [7] and 5 m/s, ignition occurs downstream over the whole range of k explored). Thus, differently from the case of $k = 1$, at $k = 10$, ignition takes place upstream (instead of downstream) and the reaction front moves one way (i.e., from upstream to downstream instead of up-and-down). Due to the absence of downstream ignition, the *burn-up* phenomenon of the residual cake, which is responsible for the maximum temperature attained during the regeneration process, occurs starting from lower temperatures. This explains why the maximum temperature decreases with increasing catalyst activity.

References

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