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Design of Engine Exhaust System for Optimum Heating of Catalytic Converter and Back Pressure Control

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ABSTRACT

Pollution from automobiles is a major source of environmental pollution and mitigating this is an important task for human health and environmental protection. Catalytic converters areimportant instruments in this regard, helping eliminate major pollutants like unburnt hydrocarbons, carbon monoxide and nitrogen oxides. Thus increasing the efficiency of catalytic converters is need of the. Catalysts of a catalytic converter become appreciably active (> 50%) after they attain a certain temperature, called the ‘light-off temperature’. Cold start emissions are extremely high before catalysts reach the light-off temperature. Therefore, minimising the time taken to achieve light-off temperature is vital. This must be done without significantly increasing the back pressure on the engine, or damaging the catalysts.Through Computational Fluid Dynamics (CFD) analysis of a simple exhaust system with a catalytic converter,it was found that light-off time is minimum when the catalytic converter is placed closest to the exhaust pipe inlet. Back pressure was found to be within tolerable limits. Steady state analysis revealed that some steady state temperatures were above 800 °C, which increases the possibility of catalyst degradation. Finally, methods (some of which have already been proposed in existing literature) have been suggested to avoid this problem.

1. Introduction

Pollution from automobiles is a major source of environmental pollution, especially in cities. Mitigating pollution from automobiles is an important task from the perspective of human health and environmental protection. Catalytic converters are the main functional instrument in this regard, which help eliminate major pollutants like unburnt hydrocarbons, carbon monoxide and nitrogen oxides. The use of catalytic converter has become necessary because of the stringent emissions protocols enforced by governments. At present, catalytic converters are very efficient in the long run. Catalysts have become efficient in the last decadesto achieve over 80% reduction[Karthikeyan et al., 2016]of the regulated pollutants, i.e. Carbon monoxide (CO), Hydrocarbons (HC) and Nitrogen Oxides (NOx), when the catalyst has reached its light-off temperature. However, they operate efficiently only at higher temperatures. These temperatures are usually attained only after the vehicles run for around 2 miles. Therefore, vehicles in cities sometimes never reach the light-off temperature, therefore always creating pollution.

1.1 Automobile Engine Emissions

Table 1 [Elliott et al., 2012] lists the major components of engine exhaust gas.

Table 1. Exhaust Gas Components

IC Engine Exhaust Gases	
Major Components (>1%)	Nitrogen
	Carbon Dioxide
	Water Vapour
	Oxygen
	Carbon Monoxide
	Hydrogen
Trace Components (<1%)	Sulphur Oxides
	Nitrogen Oxides
	Hydrocarbons
	Aldehydes
	Organic Acids
	Alcohols
	Smoke

The major components are mostly atmospheric gases, with carbon monoxide and dioxide being the only ones of concern, since CO_2(Carbon dioxide) causes global warming and CO interferes with the oxygen carrying capacity of blood[Pardiwala et al., 2011]. CO_2, however, cannot be avoided incarbon combustion based engines. The trace compounds are the more toxic emissions of Internal Combustion (IC) engines.Pollution from cars can cause several respiratory[Sinha, 1993] and other ailments and even death if inhaled in larger amounts.

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1.2 *Three-way Catalytic Converter*

The major pollutants are carbon monoxide, excess hydrocarbons and nitrogen oxides. By oxidation or reduction respectively, these can be converted to atmospheric components like carbon dioxide, water vapour, oxygen and nitrogen. However, the temperatures ordinarily required for these processes is very high. The favourable temperature for oxidization of CO and HC is reduced to 250-300°C by using catalysts. A catalyst is not consumed in the reaction so it can function indefinitely unless degraded by heat, age, contaminants, or other factors.A catalyst eases a chemical reaction by lowering its activation energy (through adsorption of reactant molecules on its surface, which makes them easily available for reaction).The reactions are the same as in regular reactors but due to inclusion of catalysts the reaction mechanism as well as temperatures varies.

The catalytic material most commonly used are platinum, palladium and rhodium. Platinum and Palladium[Pardiwala et al., 2011] promote oxidation of CO, unburnt HC, etc. into their atmospheric components i.e. CO_2 and H_2O (water) according to following reactions:

- $2CO + O_2 \rightarrow 2CO_2$
- $HC + O_2 \rightarrow CO_2 + H_2O$ (unbalanced)
- $CO + H_2O \rightarrow CO_2 + H_2$
- $HC + H_2O \rightarrow CO_2 + H_2$ (unbalanced)

Rhodium[Pardiwala et al., 2011] promotes the reduction of NOx to their atmospheric components i.e. O_2 and N_2 as shown below:

- $2CO + 2NO \rightarrow 2CO_2 + N_2$
- $HC + NO \rightarrow CO_2 + H_2O + N_2$(unbalanced)
- $2H_2 + 2NO \rightarrow 2H_2O + N_2$

At maximum efficiency, converter can remove 98-99% of CO, 95% of NOx, and more than 95% of HC from exhaust flow emissions.

The catalytic converter consists of following components:

Core/ substrate of catalytic converters can be a honeycomb structured monolith or ceramic granules. The ceramic monolith is most commonly used. Metallic foil monoliths are used in some applications. This is primarily because of the cheaper cost of large scale ceramic manufacturing. Among ceramics, Cordierite is commonly used. Among metals, ferritic steel alloys with chromium and aluminium content are used. Metallic cores are less expensive to build in small quantities.Their primary benefit is their low pressure drop. They are used inheavy duty trucks, motorcycles, high-flying airplanes, power plants etc. [Heck et al., 2001].Substrate material is designed to provide a high surface area to support the catalyst washcoat, and therefore is often called a “catalyst support”.

Properties desirable for a substrate are:

- It should be stable at high temperature.
- It should possess high ductility, toughness and shock bearing capacity.
- It should not degrade with time and temperature.
- It should not fail under thermal stresses.
- Should be inert to chemicals, water, acid etc.

The washcoat is the material that carries the catalytic materials. It enables the catalyst particles to spread uniformly over a large surface area. Aluminium oxide [Agrafiotis et al., 1999], silicon dioxide [Axelsson et al., 1988], titanium dioxide[Agrafiotis et al., 1999], or a mixture of silica and alumina [Hamill, 2011] are some possiblewashcoats. The catalysts are mixed in the washcoat prior to applying to the core. Washcoat materials form a rough surface, which greatly increases the surface area available for catalysis. The coat must retain its surface area and minimisethe sintering of the catalytic metal particles.

The catalyst is usually a precious metal. Platinum is the most active catalyst. But, it is very costly and sometimes leads to additional undesirable reactions. Therefore, it is in some cases, not suitable. Palladium and rhodium are two other examples of precious catalysts. Rhodium is used to catalyse reduction reactions, while palladium is used as an oxidation catalyst.Platinum can catalyse both the types of reactions. The other possible metallic catalysts are cerium, iron, manganese and nickel, although each has its own limitations. Nickel reacts with carbon monoxide to form nickel tetra carbonyl. Therefore, its usage is not legal in the European Union. Copper forms dioxin, therefore it is illegal in North America[Hamill, 2011].

Catalytic converters presently have a few limitations –

- Granular structured ceramics are not used much because of larger substrate volumes and thus higher massfor a given surface area [Carranza, 1999].
- The brittle nature of ceramic means honeycomb walls cannot be made too thin, because of the lack of structural strength. Thin walled ceramic structures are also difficult to manufacture compared to metallic ones.
- Washcoat bonding to a metallic substrate can be challenging due to relatively higher thermal expansion coefficient than ceramics. [Heck et al., 2001]
- Ceramic substrates are difficult to attach to the metal converter casing (Iron, Chromium, Aluminium alloys can be welded and brazed using conventional method).
- Catalysts work only in a certain temperature range. At high temperature, the noble metal catalyst particles can sinter together, reducing their effective surface area and making them less efficient.
- Lead and sulphur from fuels, and zinc, phosphorus, antimony, calcium and magnesium from oil additives can disable the catalyst.This usually occurs through the formation of a layer on the catalyst particle surface. This hampers the catalytic function of the catalysts by preventing adsorption of the reactants. This is called ‘catalyst poisoning’.

1.1 *Light-off Temperature*

The temperature at which the catalytic converter surpasses 50% efficiency is called the ‘light-off temperature’. Most common catalysts have a light off temperature of around 250 °C. The catalytic activity of the converter is very low at vehicle start-up because the catalyst temperature is low. It is very important for a vehicle to reach light-off temperature as quickly as possible to reduce the total emissions.

The light off time is affected by light off temperature of specific catalyst, temperature of exhaust gases, location of catalytic converter, specific heat capacity of the substrate, mass of substrate used, heat losses to the surrounding etc.

1.2 *Back Pressure*

Back pressure refers to pressure opposed to the desired flow of a fluid in a confined place such as a pipe. It is caused by obstructions or tight bends in the confinement vessel along which it is moving. The term back pressure is misleading as the pressure gradient remains intact and causes flow in the same direction, but the flow is reduced due to back pressure, and demands greater pressure from the pump (in this case, the exhaust stroke of engine). Back pressure caused by the exhaust system (consisting of the exhaust manifold, the catalytic converter, the muffler and the connecting pipes) opposes complete emptying of the engine cylinder. This has a negative effect on engine efficiency resulting in a decrease of power output that must be compensated by increasing fuel consumption. The back pressure depends on, pipe length, pipe diameter, pipe roughness, wall thickness of honeycomb, flow volume in substrate, substrate length, cell density of substrate etc.

2. Material and Methods

The simulations were performed using ANSYS.

The grid independence study was done using 4 different mesh sizes.

- 1.5 mm, 3 mm, 5 mm, 6 mm and 7 mm cells in different regions with boundary layer mesh.
- Standard ANSYS “Fine” Mesh with boundary layer mesh.
- 1.5 mm (in pipe region) and 3 mm (in flow region) cells with boundary layer mesh.
- 2.5 mm (in pipe region) and 6 mm (in flow region) cells without boundary layer mesh.

All 4 meshes gave negligible variation in temperature results as shown in Table 2. Thus, grid independence was established.

Table 2. Temperature Results of the Grid Independence Test

Mesh	Minimum Temperature (K)	Maximum Temperature (K)
A	1070	1098
B	1070	1098
C	1064	1099
D	1068	1099

2.1 Validation

The validation was done by comparison with the paper titled 'CFD modelling of the automotive catalytic converter' [Hayes et al., 2012].This was also used to find suitable porous resistance parameters.The validation was done with a 2D planar geometry, as was done in the concerned research paper. The angles of diffuser and nozzle were kept constant. The diameters of both the pipe and the substrate were kept constant, while the length of the substrate was varied as shown in Figure 1a.

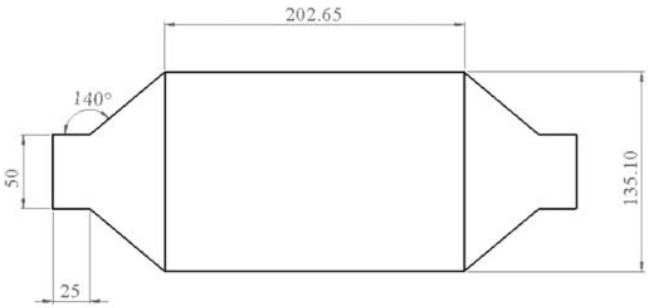

Figure 1a. Sample geometry used for validation. Cylinder length was varied.

The meshing was done with ANSYS Workbench and analysis was done in ANSYS Fluent, whereas the original paper used COMSOL. The standard "Coarse" mesh size defined in ANSYS was used, after studying the grid independence. The mesh also included boundary layer mesh with 5 layers having a growth rate of 1.5 and a total thickness of 5 mm (Figure 1b).The boundary conditions and other parameters were same as reference paper.

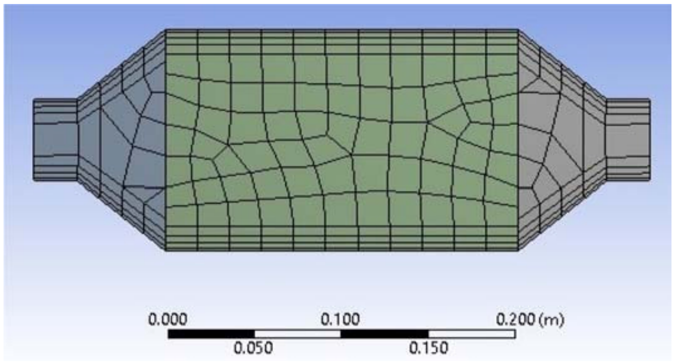

Figure 1b. Mesh used for validation

Validation of flow characteristics was done by trying to replicate the results of a research paper. Keeping the diffuser angle and diameter constant, various flow rates were simulated through a porous medium, for different lengths of porous medium. The resistance values were suitably decided and the pressure drop results were compared. Comparable results of reference and current study shown in Figure 2 validates the selected model.

2.2 Geometry Selection

It had to be decided which type of geometry was to be used. The choice was between the actual 3D geometry or a small sector of the 3D geometry (30° angle) or a 2D planar geometry for ensuring accurate results in optimum simulation time. The advantages of the 2D geometry include significantly lower calculation time. Whereas the disadvantages include lower accuracy due to the approximations involved in making a 3D model into 2D. The sector model was thought to be a compromise, with the accuracy of a 3D model, but higher computation speed due to lower number of cells.

Therefore, all three models were simulated and their temperatures and pressures compared in steady state (Table 3).

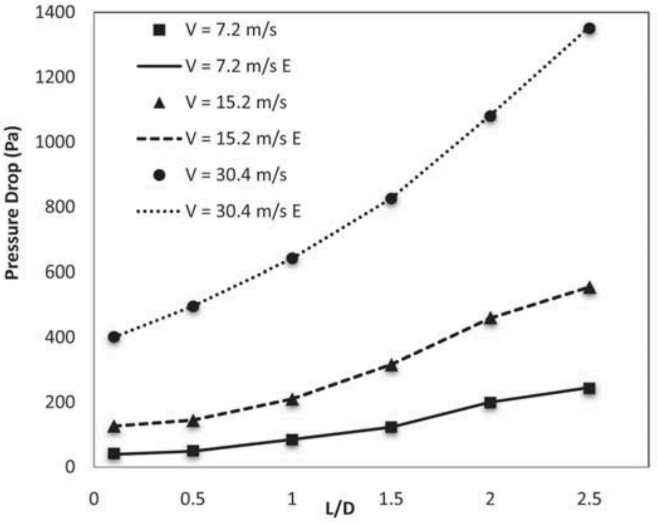

Figure 2. Results of validation; the lines (suffixed "E" in legend) denote reference results, the points denote our results.

Table 3. Results of Geometry selection tests

Geometry Type	Sector	3D	2D
Volume Average Temperature (K)	905.27	906.4	1008.48
Maximum Temperature (K)	1053.53	1038.57	1082.56
Minimum Temperature (K)	682.98	692.66	743.84
Pressure Drop (Pa)	824.75	789.25	931.54

The (Perimeter/Area) ratio of the 2D model is lower than the (Surface Area/Volume) ratio of the 3D model. Therefore, 3D model showed greater convective cooling, hence lower temperatures. Similarly, flow area in 3D increases as square of diameter, whereas in planar 2D, it increases linearly. Therefore, velocity after the diffuser is lower for 3D, leading to lower pressure drop than 2D.

Because of the significant differences in results of the three geometries, it was decided to use the full 3D model.

2.3 Main Simulations

In this investigation, multiple geometries were made using different inlet lengths according to parameters shown in Figure 3a. The geometry included only the flow region and not the solid pipe, since the convection boundary condition taken from literature was already suitably adjusted for the thermal resistance of pipe. This enabled us to reduce the number of mesh cells considerably. The model consisted of inlet pipe, diverging section, porous region, converging section, and outlet pipe.

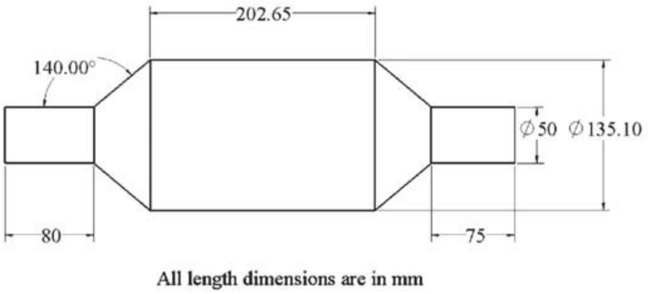

Figure 3a. Sample geometry for transient analysis. Inlet pipe length varied.

The meshing was done in ANSYS Workbench. The standard mesh size “Medium” predefined in ANSYS was used. A 5 mm boundary layer mesh was created with 5 cell layers and a growth rate of 1.5 for each consecutive layer. A sample mesh is shown in Figure 3b.

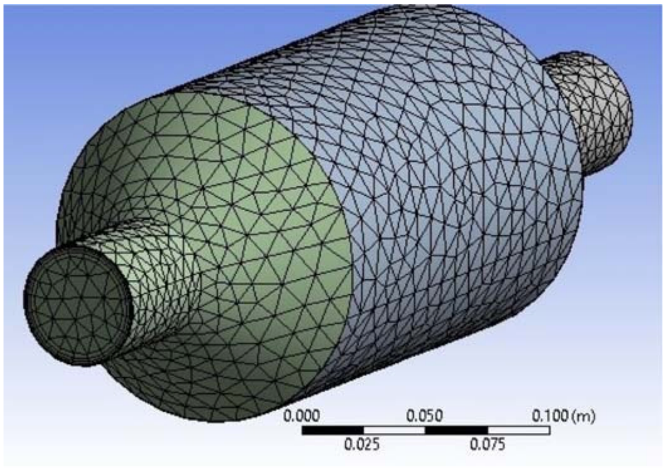

Figure 3b. Sample mesh for transient analysis

In the simulation parameter selection, the transient energy equation was activated. The “realisable K-epsilon turbulence” model with “scalable wall functions” was used. For material properties three materials were used. Cordierite was used for the ceramic substrate, with the density 556.5 kg/m^3, specific heat capacity 1464.4 J/kg-K and thermal conductivity 3 W/m-K. The fluid was assumed to be air, taken by default from the ANSYS database to have density 1.225 kg/m^3, specific heat capacity 1006.43 J/kg-K, thermal conductivity 0.0242 W/m-K and viscosity 1.78e-05 kg/m-s. For the metal substrate, ferritic steel was assumed with specific heat 460 K/kg-K and thermal conductivity 25 W/m-K. The original density of the metal is ~7700 kg/m^3. However, to mimic the thermal effect of the thinner walls that are possible with a metal substrate, without changing the porous resistances, we reduced the density of the metal to 556.5 kg/m^3.

Inlet velocity was calculated to be 11.83 m/s corresponding to 800 CC engine operating at 3500 RPM according to parameters specified in Table 4. Inlet temperature of exhaust gases was assumed to be 1100 K. Pressure outlet was defined at atmospheric conditions.

Table 4. Calculation of exhaust velocity

Engine Volume	0.796	L
Engine Speed	3500	RPM
Exhaust strokes / s	29.167	s^{-1}
Volume flow rate	23.217	L/s
Pipe Diameter	0.050	m
Area	0.002	m^2
Flow Velocity	11.830	m/s

Convection boundary was applied to the walls with a coefficient of 14.9 W/m^2-K and an ambient temperature of 300 K. These values were taken from the paper used for validation [Hayes et al, 2012]. Porosity was taken to be 0.62, with the viscous resistance coefficient being 9.15e+06 and the inertial resistance coefficient being 8.91. Area density of the porous substrate was taken to be 2479 m^2/m^3, and the total heat transfer coefficient as 1.5.

After meshing, a Non-equilibrium porous region mesh was constructed in Fluent. This “solid” mesh is coincident with the original “fluid” porous region mesh. The two meshes only exchange thermal energy. Geometry, porous region conditions and convection boundary conditions were taken from the validation literature. Several transient simulations were carried out with varying parameters. The porosity was held constant. The length of the inlet pipe was varied from 2.5 cm to 60 cm. The time required for the average substrate temperature to reach light-off as well as the time required for the minimum substrate temperature to reach light-off was noted. The same simulations were then carried to steady state, and steady state temperatures and back pressures across substrate were noted. Effect of reactions in a cold catalytic converter (before light off) were negligible. Therefore it has little effect on light-off time. So, we did not consider the heat of reaction in our simulations. Finally, one simulation was conducted using a metallic substrate. Metal substrates can be much thinner and smaller than ceramics. They have lower specific heat capacity but higher density. However, we wanted to consider only the effects of its thermal properties without changing porous parameters. Therefore, to approximate the thermal effect of thinner walls, we reduced the effective density of the metal instead of changing the geometry and porous parameters.

Simulations were also carried out for metallic substrates and results are compared with ceramic substrates

3. Results and Discussions

Figure 4 shows the variation of time requirement to attain light-off temperature with inlet pipe length. As the length of the inlet pipe increases, convection losses through the pipe increase. Therefore, colder exhaust air reaches the converter, and the time required for the converter to get hot increases. The minimum light off time is observed at the smallest inlet pipe length that we used, i.e. 2.5 cm.

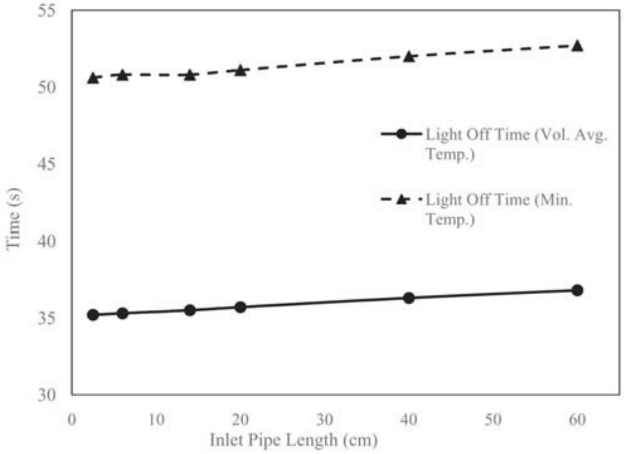

Figure 4. Time required to attain light-off temperature; triggered by average temperature and minimum temperature

As the length of pipe increases, the steady state temperatures decrease (Figure 5). This is due to increasing convection losses in the inlet pipe. The thermal degradation of the catalytic converter begins at around 800-900 °C. As we can see, even up to 60 cm inlet pipe lengthmaximum steady state temperature reacheswithin this range. This can potentially damage the catalysts, hence needs to be avoided. There could be several methods used to reduce this maximum temperature.

The pressure drop across the catalytic converter is approximately independent of the inlet lengths (Figure 6). Similarly, the back pressure at the inlet has an approximately linear dependence to the total pipe length (the outlet pipe length of the model is constant), as is expected.Since the total pipe length in a car can be expected to be independent of the converter placement, we can seethat the placement of the catalytic converter has no significant effect on the back pressure. Hence, only light off times and maximum steady state temperatures can be considered while deciding the optimal placement of catalytic converter.

Table 5 show the comparison between metallic and ceramic substrates. Metallic substrates can be made with much thinner walls than ceramic substrates, thus reducing the solid volume in the porous region. This, coupled with their lower specific heat and higher thermal conductivity ensures that metal substrates get heated very quickly. The higher thermal conductivity also ensures that steady state temperatures for the metallic substrate are lower. This lowers the chance of thermal degradation of catalysts.

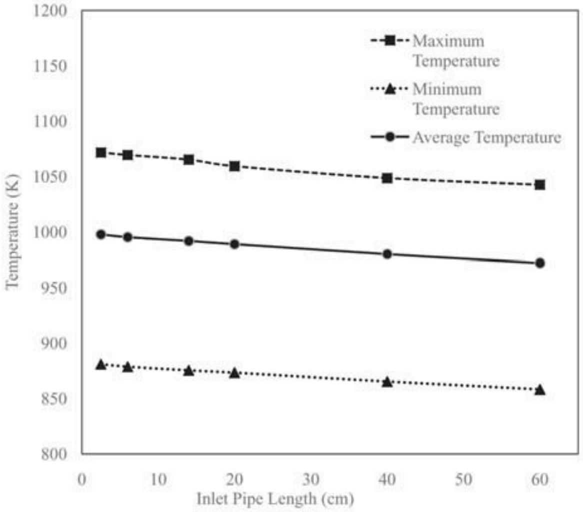

Figure 5. Steady state temperatures variation with inlet pipe length

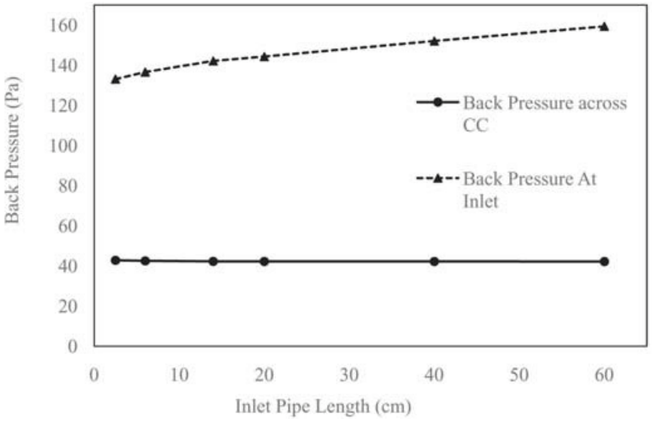

Figure 6. Pressure drop across the porous region and across entire pipe; variation with inlet pipe length

Table 5. Comparison between ceramic and metallic substrates

Parameter	Ceramic	Metallic
Light-Off Time (Volume Average Temp.)	34.5 s	11.2 s
Light-Off Time (Minimum Temp.)	47.1 s	13.3 s
Maximum Steady Temperature (K)	1090.28	1007.14
Minimum Steady Temperature (K)	1065.32	957.8
Volume Average Temperature (K)	1081.54	984.4

4. Conclusions

The minimum time to attain light-off temperature occurred with minimum length inlet pipe (considering both average and minimum temperature times). The pressure drop across porous zone is independent of its placement. The overall pressure drop is well within tolerable levels.

Thus, the optimum inlet pipe length for attaining light off temperature quickly seems to be the minimum length that is possible.

However, smaller inlet pipes leads to higher steady state temperatures and risk of thermal catalyst degradation. Therefore, the catalytic converters are usually placed further behind compared to the ideal length. Therefore, there is a need for reducing the maximum temperature in the converters. Several methods could be used for this. Some are listed below.

Metallic substrates: One option we explored in our simulations was metal substrates. Metallic substrates can reduce all our problems simultaneously. As we have seen through simulations, metal substrates have better light off times than their ceramic counterparts. At the same time, the higher thermal conductivity leads to better heat transfer out of the substrate and hence, lower steady state temperatures. The possibility of thinner walls means that pressure drops across the converter can be reduced. Metal substrates are also easier to manufacture and can be made in a variety of sizes and shapes, whereas large ceramic substrates are difficult to make. Possibility of recycling the metalsadds to the desirability. Thus, metal substrates have significant advantages over conventional ceramic substrates. Their only apparent disadvantage is their higher cost.

Other methods can be tested through simulations in the future. Following methods proposed in the literature can be further explored for improvement in the efficiency and durability of catalytic converters.

Multiple Pipes: After the catalytic converter reaches light off, the exhaust gas can be taken on a detour through a much longer pipe to limit the maximum steady state temperature, while exothermic reactions sustain light off temperature. This can cool the exhaust gas sufficiently through convection with environment before being channelled into the catalytic converter. However, the resultant increase in back pressure and its effects could be analysed.

Thermoelectric generator[Yang et al., 2006]: After the catalytic converter surpasses light off temperature, the exhaust gas can be diverted through a thermoelectric generator to cool it before sending it into the catalytic converter, as shown in literature. This will also generate some energy that could be stored in the battery, while simultaneously reducing the maximum steady state temperature.

Heating methods[Kinnear and Baccarini, 1992; Crawford and Douglas, 2015; Reddy, 2015]: The inlet pipe can be made longer to limit the maximum steady state temperature.Alongside, various temporary heating methods as seen in the literature (Joule heating, electromagnetic induction heating, chemical heating, etc.) can be used to directly heat the catalytic converter to reduce the cold start period.

Insulation methods [Burch et al., 1994; Burch et al., 1995]: It has been suggested to use vacuum insulation to prevent heat loss from the catalytic converter when the vehicle is off, so that the catalysts do not have to go through cold start the next time the vehicle is started. During operation, hydrogen gas is injected in the vacuum chamber in a controlled manner to enable conduction and prevent overheating.

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