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Regeneration Of Diesel Particulate Filters With Hydrogen Rich Gas*

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Abstract

The options for the regeneration of a Diesel Particulate Filter (DPF) using hydrogen rich gas are investigated. The advantages of using hydrogen rich gas for this purpose are described. The system requirements for such a system are also evaluated. The use of a plasmatron fuel converter for the onboard generation of hydrogen rich gas from diesel fuel is discussed. The advantages of homogeneous, non-catalytic reforming by the plasmatron fuel converter are described. Finally, the effect of homogeneous combustion of the hydrogen rich gas in the exhaust (upstream from the DPF) is investigated.

I. Introduction

Particulate and emissions from diesel vehicles have been determined to be hazardous to health. In addition, particulate emissions may aid to the global warming trends because of the reduced reflectivity of large masses of ice/snow. Diesel emissions have been regulated in the developed countries. Tighter regulations already in the books require substantially decreased emissions in the next 5 years.

A promising technology to accomplish the required reduction is the Diesel Particulate Filter (DPF). The filters are porous ceramics through which the gases flow relatively unimpeded, but the solids in the exhaust are trapped. Eventually there is sufficient buildup of the particulates in the trap that the gas flow is impeded, and regeneration needs to take place.

Two types of traps exist, with or without a catalyst coating. Uncoated DPF are attractive because of reduced cost, and because it is likely that some method of active regeneration will be required even if used rarely. The uncoated DPF need to be regenerated by the combination of temperature and oxygen. Combustor technology has been developed. However, there may be important advantages to regenerate the DPF using hydrogen rich gas, in which the reformate is combusted in the trap itself, hopefully by the soot. The potential advantages are reduced thermal stress, lower temperature of trap regeneration, reduced possibility of uncontrolled regeneration that may result in the destruction of the trap and lower fuel penalty by the use of controlled burn. These advantages may result in enhanced reliability and increased lifetime. For both catalyzed and non-catalyzed traps, there has to be sufficient oxygen in the flow through the DPF in order to combust the soot. For any active regeneration method, the system should be able to operate over a wide range of non-stationary conditions.

In order to "ignite" the particulate matter, it has also determined that a temperature in the range of 600-650 C was required in the presence of oxygen. Measured activation energies varies from ~60 kJ/mol to 170 kJ/mol. The temperature rise of the gas across the DPF (and the temperature of the DPF unit) depends on the oxygen content, the mass loading of the field and the flow rate. The temperature excursion due to the soot combustion can be as low as a few degrees to high temperature excursions that can result in the destruction of the trap.

Two modes of regeneration have been observed in uncatalized traps. Visual evidence of the mode modes has been obtained by Haralampous. The first mode results in a uniform regeneration of the trap, with mild temperature excursions and relatively long regeneration times because of the low temperatures. This mode of regeneration built in margins, results in a more uniform regeneration, but increases the fuel consumption due to the fact that the temperatures need to be maintained longer, in the case of non-self-sustaining regeneration. The second regeneration mode results in a self-sustained or near-self sustained burn, with higher temperatures, non-uniform and faster regeneration (in some cases resembling a propagating front). The nature of the regeneration process is

determined mainly by the trap soot loading, the free oxygen content of the exhaust and the exhaust flow rate.

In the second mode of operation the regeneration is performed by increasing the temperature of the exhaust to the point where the soot ignites and starts a self-sustaining burn. Once started, it is uncontrolled. If there is too much soot in the trap or if the free-oxygen concentration is increased (from lower torque operation, for example) the temperatures of the combustion process can exceed the temperature limitations of the filter. A single event may result in unintentional destruction of the filter.

Low temperature regeneration may result in more uniform regeneration. Non-uniform regeneration that results in partial regeneration of the DPF has been modeled and tested by Haralampous et al., and others. The flow through the DPF, even if uniformly loaded, changes during regeneration. If some regions are cleaned prior to others, the flow pattern downstream of the clean channel can be substantially modified, with an increasing fraction of the flow occurring through the clean region. Non-uniform channel regeneration affects both the radial and axial flow patterns. Axial flow pattern maldistribution occurs when the upstream region of a channel is cleansed faster, after which the gas flows across the cleansed region instead of the downstream, soot-loaded channel.

The first mode of operation is attractive in that the rate of combustion, and the temperature of the regeneration process, is dominated by the exhaust gas and not by the self-sustained combustion of the soot. From the above discussion, low temperature, slow uniform regeneration has attractive features.

Tests with active regeneration are taking place both in the US [Donaldson] as well as in Europe [Fayard]. Active techniques at present seem to be necessary for those vehicles with substantial idling, where the exhaust temperatures are too low for self-sustained DPF regeneration. These concepts depend on thermal management to increase the temperature of the DPF, as well as active introduction of fuel upstream in the exhaust. The fuel is injected upstream from a diesel oxidation catalyst (DOC) that is located upstream from the trap. The fuel is consumed in the DOC, increasing the temperature of the exhaust. The oxygen content downstream from the DOC is sufficient for soot combustion.

Alternative methods to the catalytic combustor involves a conventional combustor. This technology is being tested by Arvin Meritor.

Fuel reformers are being considered for on-board applications, for hydrogen generation for use with fuel cells, for use in NOx trap regeneration, and for combustion improvement in SI engines. The MIT team is developing plasmatron fuel reformers, both for gasoline and diesel applications. Both catalytic and homogenous reformers are being investigated. Plasma based reformers are robust, fast response and have wide operating capability. It is the purpose of this paper to investigate options of using reformate from a plasmatron fuel reformer for the controlled regeneration of DPFs.

II. Plasmatron Technology for DPF Regeneration

Active techniques for the regeneration of diesel particulate filters use a burner to achieve the temperatures at the catalyst required for filter regeneration. Plasmatron technology can be used as a fuel igniter as well as means to produce hydrogen rich gas. Plasmatron technology can serve as a powerful igniter and thus is attractive because it is possible to combust the diesel fuel using oxygen present in the diesel exhaust, even at conditions when the engine is operating at high load (with reduced oxygen content). Diesel loads rarely operate above equivalence ratios around 0.7, because of soot production, and thus about 1/3 of the oxygen remains free in the exhaust.

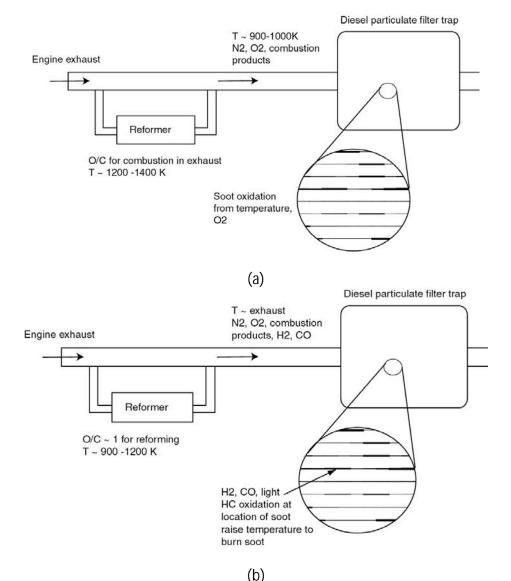


Figure 1. Reformer operating as a (a) combustion for DPF regeneration (b) Generation of hydrogen rich gas

By using the plasmatron unit as a powerful igniter, either very lean mixtures or very rich mixtures can be processed. Very lean conditions can occur when only the thermal process of the fuel is desired. Rich conditions will result in the generation of hydrogen rich gas.

The advantage of combusting the fuel in the exhaust is that it is possible to achieve combustion while minimizing the amount of extra air introduced into the system. The hydrogen rich gas with exhaust gas as oxidizer results in a further net decrease of the amount of free oxygen in the exhaust, decreasing the combustion rate of the soot on the DPF and decreasing the possibility of uncontrolled regeneration. This technology is also attractive because the plasmatron hardware may already exist on-board the vehicle for regeneration of NOx absorber traps.

Figure 1 (a) shows a schematic of the use of a reformer as a powerful combustor, operating with exhaust as the oxidizer. There is thermal output from the combustor, but no hydrogen or light hydrocarbons. In figure 1(b) the reformer operates under conditions close to partial oxidation (free oxygen to carbon ratio of 1), producing hydrogen, CO, light hydrocarbons and limited thermal output (~ 1/4 of the thermal output of the fuel is combusted in the reformation process). These two are extremes, with the plasmatron operating anywhere in between, generating both easily combustible gases as well as thermal output.

Two options of location of the DPF and NOx trap exist. The DPF can be upstream from the NOx trap, or the other way around. Modeling of the system is required to determine the optimal configuration. Care must be taken that the temperature required for regeneration of the DPF does not damage the NOx trap, as well as the issues having to do with desulfation of the NOx trap.

III. Calculations of Reformer Requirements

For the calculations presented here, the size of the engine is 6 l, operating between 600 and 2400 rpm, with a inlet manifold pressure of 1-3 bars, It is assumed that the entire exhaust flow is treated, as opposed to partial regeneration of a section of the DPF [Bromberg].

The exhaust temperature assumed throughout the engine map is shown in Figure 2. For simplicity, it is assumed that the exhaust is insensitive to engine speed and only depends on torque.

It is assumed that the soot burns at temperatures between 600- 700 C. The reformate is mixed with the exhaust to increase the temperature to this range. The flow rates through the plasmatron are calculated, at different O/C ratios.

Because the reformate is combustible, the rates that are calculated will be larger than those actually required. The actual flow rates will thus be lower.

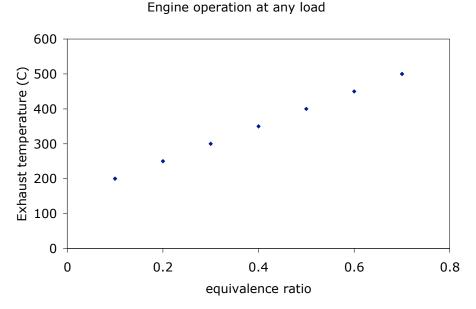


Figure 2. Exhaust temperature as a function of the engine equivalence ratio. It is assumed that the exhaust temperature is insensitive to the engine speed.

In addition, it is assumed that turbocharging does not increase the temperature of the exhaust, due to the presence of an intercooler.

Two scenarios for the regeneration with hydrogen rich gas can be envisioned. The first one assumes that it is the thermal content of the hydrogen rich gas that results in the regeneration of the DPF. In this manner it does not really matter where the hydrogen rich gas is combusted. The second scenario assumes that the hydrogen rich gas reacts in the region of the soot (and even is ignited by the soot), resulting in direct deposition of the heat at the soot location. In this scenario, the temperature of the exhaust is low prior to the combustion of the hydrogen rich gas, and thus the velocity of the gas is slower, allowing for increased contact time between the free oxygen and the hydrogen rich gas with the soot. In the second scenario, it is desired that the hydrogen rich gas not be consumed homogeneous prior to the region with the soot. Homogeneous combustion of hot hydrogen rich gas in the exhaust is discussed in the section below.

In both scenarios, the temperature of the gas, assuming combustion of the hydrogen rich gas, is ~ 600 C, thus able to start regeneration of the soot. Because of the light soot loadings assumed, the temperature downstream from the soot is not significantly larger than upstream (*i.e.*, the soot is burning at a low rate).

The reformate power required to bring the temperature of the exhaust to regeneration conditions in the DPF is shown in Figure 3. The reformate power refers to the combustion power if the reformate is fully oxidized. The power increases linearly with speed, at any equivalence ratio. The reformate power also increases with decreasing equivalence ratio, as the exhaust temperature prior to addition of the reformate is cooler

in the cases of low equivalence ratio, and thus increased reformation is required to achieve the regeneration temperature.

The range of power is large, from a minimum of ~ 3 kW to about 30 kW, for a dynamic range of ~ 10 . However, this is larger than it need be, since the engine will not work often the region of high rpm and low torque. Thus, the dynamic range requirements are ~ 5 . This dynamic range does not include operation at higher manifold pressure, discussed below. It is the possibility of operating a plasmatron over this wide range of condition that makes it attractive for the DPF regeneration application.

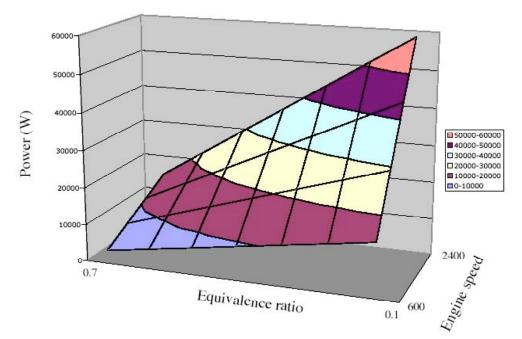


Figure 3. Power in reformate (rate of heating value, in Watts), required for reaching regeneration conditions, as a function of the equivalence ratio and the engine speed, for naturally aspirated conditions.

Figure 4 shows the fuel flow rates through the plasmatron for achieving regeneration through the engine map for the case of 3-bar operation of the engine (with an intercooler). The behavior is very similar to that shown in Figure 3 for naturally aspirated engine, with the largest fuel flow rate requirements at high speed, low torque. The highest fuel flow rate through the fuel processor is 5 g/s, which corresponds to a maximum power of about 160 kW. However, the engine is unlikely to operate under conditions of high speed, low torque and high manifold pressure. Thus, turbocharging does not result in substantial changes in the required dynamic range from the fuel processor.

The time required for regeneration is determined by the PM burn rate, which depends on the temperature and oxygen concentration. The effect of the hydrogen rich gas is unknown and will be determined in the experiments. Calculations of combustion rate of the soot can be made using the Arrhenius formulation with the activations energies described above, but cannot be used as a predictive tool. The development of plasmatron fuel reformers demonstrated the capability to operate from about 0.3 g/s to 2 g/s, with activities to achieve 4 g/s fuel flow rate. Most of this work has been carried out with gasoline, but could be extrapolated to diesel. Thus, the capabilities of the present devices match the requirements for DPF regeneration.

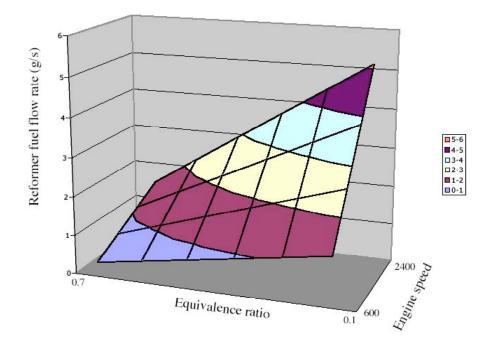


Figure 4. Rate of fuel flow rate through the reformer (in g/s) required to achieve regeneration conditions as a function of the equivalence ratio and the engine speed, for 3-bar inlet manifold pressure.

IV. Testing Procedure

Testing will be carried out in using an '02 Cummins ISB 300 5.9L inline 6 engine. The engine characteristics are: maximum power ~ 225 kW, maximum torque ~ 895 N•m, compression ratio: ~17, bore diameter: 102.02 mm and piston stroke: 120 mm. The engine setup is described elsewhere.

The cordierite DPFs to be tested were obtained from Corning. They are conventional units 5.66 in diameter, 10 in long traps with a cell density of 100 cpsi.

Full trap and partial traps will be tested. For full trap, the entire trap will be loaded and regenerated, maybe with multiple units. Partial traps will be constructed from 2 in diameter sections of the trap. Experience indicates that if 5 cm (2 in) sections of the PDF are used, the edge effects are not important [Ogonwumi]. Using partial trap allows for quicker soot loading, facilitating the tests in a wider range of conditions.

The engine produces a raw exhaust with a PM emission of 0.1 g/kW hr. A 5 cm diameter (2 in) partial unit is about 1/32 of the volume of a DPF that consists of 4 14.4 cm diameter (5.66 in) units. The volume of the partial unit is on the order of 0.3 liter, while the single trap is about 2.5 liters. Typical loadings on traps prior to regeneration are on the order of 10 g/liter. Thus, the time required in order to load the partial unit, at 40 kW (50 hp), is 45 minutes, if all the flow is through the partial unit. Forcing all the flow through a single partial unit may, however, result in large pressure drop.

It should be noted that it has been determined that the loading rate of the trap is important, as the loading of the soot is nonuniform at the higher loading rates [Staerker]. At the high flow rates (320 kg/hr) through the trap, the particle trap experienced loading that peaks off-axis, while at lower exhaust flow rates of 60 kg/hr the soot is deposited uniformly. This is counterintuitive, because at the higher flow rates the Reynolds number is higher and thus increasingly turbulent, which results in a uniform flow profile (but increasingly non-uniform soot profile in the trap).

In order to load the single full unit, at the same engine loading, it would take over 2 hours. Although acceptable, partial units would allow the quick exploration of a large set of parameters.

The present plans call that, after trap loading, a reduction in the flow through the partial unit to the nominal flow. The partial trap will be regenerated from hydrogen rich gas provided from bottled gas.

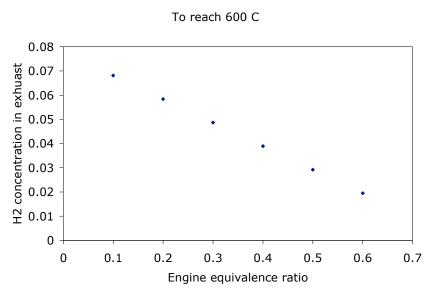


Figure 5. Hydrogen concentration in exhaust if reformate reaches equilibrium in the reformer, as a function of the engine equivalence ratio.

To regenerated the DPF at 1200 rpm, half-torque conditions, about 20 kW of reformate are required. Since the flow through the partial unit is 1/32 of this, only about 0.5 kW of

reformate is required for the regeneration. This corresponds to a reformate flow rate of 0.2 cfm. With a 300 ft³ bottle, tests can be carried out for 24 hours of regeneration.

If instead a trap with a single 5.66 in DPF is used, the flow rates would be 8 times larger, and the bottle of gas would be consumed in about 3 hours.

After the testing with the partial unit, with some optimization of the process, tests with a full unit or multiple full units can be carried out. The process would require long periods for time for loading the trap with PM, followed by regeneration.

The hydrogen gas from the plasmatron is by nature hot, on the order of 800 - 1000 C. Because of finite mixing in the exhaust, some of the gas will retain its hot temperature, making it more ignitable by the warm soot particles. To test the effect of temperature, the reformate will be heated using electrical heaters. Again, the reduced flow rate would help in the design of the heaters. In order to preheat the gas to those temperatures, approximately 100 W of electrical heating needs to be provided. This will be done in the absence of oxygen.

Finally, it should be mentioned that in the homogeneous plasmatron fuel reformer, the reformate does not reach equilibrium. Thus the concentration of hydrogen in the case of a homogeneous plasmatron reformer is about 1/3 that of equilibrium, or about 8%. The rest of the hydrogen in the fuel is converted to light hydrocarbon, such as methane and ethylene, that are also relatively easily ignitable (combust with low production of soot). The advantage of this is shown in Figure 5 which shows the concentration of hydrogen in the reforming reaction reaches equilibrium, if well mixed with the exhaust. If the reforming reaction reaches equilibrium, the concentration of hydrogen reaches explosive limits in the exhaust, especially at the lower engine equivalence ratio, when the oxygen excess is maximum. However, by operating a non-equilibrium reformer and decreasing the concentration of hydrogen in the reformate, the explosive conditions are avoided.

V. Homogeneous Oxidation of Reformate in the Exhaust

In this section, the issue of hydrogen oxidation in the exhaust is considered, to determine whether hot hydrogen-rich gas injected into the exhaust (that contains free oxygen) will spontaneously combust prior to reaching the trap.

a) Model

For simplicity, it is assumed that the 6 liter engine operates at 600 rpm, and that it is operated at idle (at an equivalence ratio of 10%, without EGR). Thus, the concentration in the engine exhaust is 18.7% O_2 , 78.2% N_2 , 2% H_2O and 1% CO_2 (assuming methane as the fuel). To this exhaust, which is assumed to be at 423 K (150 C), hydrogen rich gas is injected. These conditions correspond the worst case, with the highest amount of free oxygen and the largest demand of hydrogen rich gas. In this section it is assumed that the hydrogen rich gas is the result of equilibrium partial oxidation of methane, at different

O/C ratios. Methane is used because of the existence of chemical reaction mechanisms that have been benchmarked for operation at the fuel-rich conditions of the reformer.

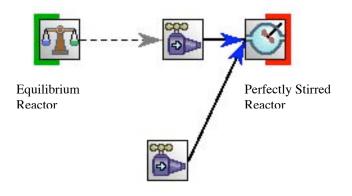


Figure 6. Schematic model of the process

The model is schematically shown in Figure 6. It is assumed that the equilibrium reactor and the exhaust are introduced into a perfectly stirred reactor (PSR). A model that uses a plug flow reactor is described below, but the constrains of the code made the assumption of the perfectly stirred reactor easier to input. The model shown in Figure 6 overestimates the consumption of hydrogen, since as the hydrogen is consumed, the PSR model implies that the temperature upstream from the reactor increases, driving additional hydrogen consumption. The goal is to determine the conditions for which the exhaust will result in substantial amounts of hydrogen oxidation. A more detailed model will be presented in a section below.

The conditions chosen correspond to about 40 g/s exhaust gas, with 10 g/s from the reformate (corresponding to about 1.5 g/s fuel in the plasmatron). This is a large number, but the goal is to determine under the worst of conditions, what is the effect of the hydrogen combustion

b. Results from the PSR Model

Three cases have been assumed, with oxygen to carbon ratios of 1.333, 1.43 and 1.54. They correspond to methane flow rates of 1.5, 1.39 and 1.29 g/s, for a total flow rate of 10 g/s.

| Table 1. Results for the PSR case | | | | | |
|-----------------------------------|-----------------|--------|-------|-------|-------|
| | O/C | | 1.33 | 1.43 | 1.54 |
| | Fuel flow rate | g/s | 1.49 | 1.39 | 1.29 |
| | T equil reactor | K | 1157 | 1255 | 1359 |
| | T exhaust | K | 423 | 423 | 423 |
| | T PSR | K | 628 | 654 | 1489 |
| | | | | | |
| | PSR H2 input | mols/s | 0.164 | 0.147 | 0.130 |
| | PSR H2 out | mols/s | 0.164 | 0.147 | 0.001 |
| | | | | | |

The results are shown in Table 1. T equil reactor represented the temperature from the equilibrium reactor, and it is the equilibrium temperature of the partial oxidation reaction. The temperature of the exhaust is held constant at 423. T PSR represents the temperature of the perfectly stirred reactor (and the outlet from that reactor).

For the first two cases, with relatively low O/C, the hydrogen flow rate out of the PSR reactor is approximately the same as the hydrogen rate into the PSR. That is, there is no oxidation of the hydrogen in the flow rate. The same is the case for the CO that is also produced. The last case, though, with a relatively high O/C, results in almost all consumption of the hydrogen rich gas. The temperature of the system becomes very large, as the hydrogen rich gas has substantial thermal content, increasing the reaction rate of hydrogen. There is oxidation at reformate/exhaust temperatures exceeding 700 K.

This case represents the most pessimistic and unrealistic case, since it requires substantial mass and temperature equilibration in the exhaust pipe. This flow resembles more the plug flow model, which will be described next.

c. Plug Flow Reactor Simulation

In this section, an alternative reactor is used as a model. This reactor simulates more closely the processes inside the system. The PFR is a more appropriate model for the behavior of the hydrogen rich gas in and environment with free oxygen in the exhaust of a vehicle.

The model is shown schematically in Figure 7. It includes, as in the previous section, an equilibrium reactor that represents the reformer, a second input to the PSR that represents the engine. The PSR is used with very short residence time (0.001 s) as a mixing, nonreacting reactor. The PSR is then followed by a plug flow reactor (PFR). It is assumed that the PFR has a diameter of 5 cm (2 in) and a length of 30 cm (12 in). This distance corresponds to the length between the injection point of the hydrogen rich gas in the exhaust and the aftertreament unit. In this case, the amount of reformate is decreased to 3 g/s (down from 10 g/s in the previous section), with an O/C ratio of 1.33.

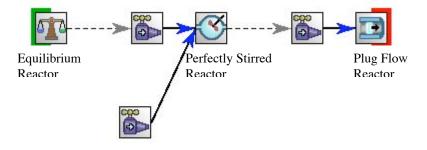


Figure 7. Schematic diagram of model for hydrogen oxidation in exhaust pipe.

The temperature of the exhaust is varied, until there is homogeneous reaction (i.e., combustion) in the exhaust. A case just above the temperature at which the air/fuel mixture ignites is shown in Figures 8 and 9. Figure 8 shows the temperature of the reformate/exhaust gas as a function of the distance along the plug flow reactor, when the temperature of the engine exhaust is 973 K.

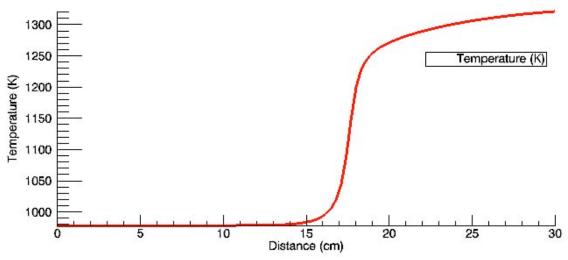
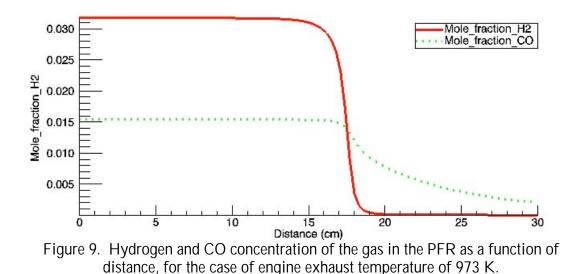


Figure 8. Temperature as a function of distance in the PFR, assuming that the engine exhaust is at 973 K

Half way along the exhaust pipe the fuel (hydrogen rich gas) ignites. The corresponding composition of the reformate/exhaust gas is shown in Figure 9. It is interesting to note that hydrogen burns faster than CO.



For an exhaust temperature of 923 K (i.e. 50 K lower than the temperature for which the hydrogen rich gas ignites), there is no reaction in the length of the PFR. The hydrogen and CO concentrations remain the same to within 3 significant digits.

The temperatures required for ignition of the hydrogen rich gas are substantially higher than those commonly found in the operation of diesel engines. Thus, it is not thought that hydrogen rich gas from an equilibrium reformer will combust homogeneously in the exhaust.

d. Non-Equilibrium Reformer

The last case uses the experimentally derived concentrations for a homogeneous plasmatron operating on diesel, utilizing the PFR described in the section above. The model is described in Figure 10. It is assumed that the concentration of the reformate is $8\% \text{ H}_2$, 10% CO, $3\% \text{ CH}_4$, $1\% \text{ C}_2\text{H}_6$, $4\% \text{ CO}_2$, $6\% \text{ H}_2\text{O}$ and $68\% \text{ N}_2$. These numbers are typical of operation of the generation 3 plasmatron. In addition, it is assumed that the temperature of the reformate prior to mixing with the exhaust is 1100 K. The flow rates are the same as with the PFR (3 g/s of reformate and 40 g/s of exhaust).

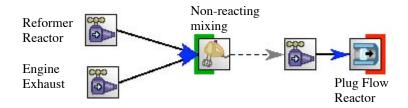


Figure 10. System without equilibrium reactor for reformer.

As in the previous section, the temperature of the engine exhaust is varied until there is combustion in the exhaust pipe. It is found that the temperature of engine exhaust has to be increased to 1073 in order to see ignition of the reformate/exhaust flow. Results at this temperature are shown in Figures 11 and 12.

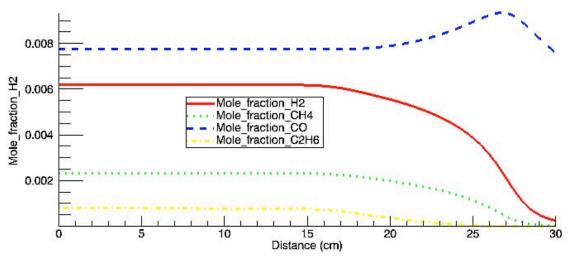


Figure 11. Concentration in exhaust as a function of distance for an exhaust temperature of 1073 K, for reformer composition similar to that of present day homogeneous plasmatron reformers.

At an exhaust temperature of 1073, there is combustions. At 50 K lower temperature, there is no reaction at all. The temperature profile is shown in Figure 12.

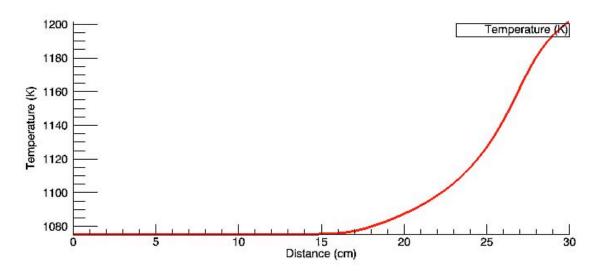


Figure 12. Temperature corresponding to the case in Figure 11 as a function of distance

The ignition conditions of the non-equilibrium reformate requires engine exhaust temperatures comparable to the temperature of the reformate. The temperature in this case is even higher than that described above for the equilibrium reformer, and they are not reached in normal operation of a diesel engine.

The results indicated in this memorandum are for homogeneous (gas phase) reactions. The object is that the hot carbon particles can induce combustion of the hydrogen rich gas locally, substantially increasing the particulate temperature and thus the combustion of the particulates.

VI. Conclusion

Reformate requirements for achieving DPF regeneration have been calculated on the basis of simple models. It has been determined that the flow rates requirements for a 6 l turbocharged engine, are within the range of today's plasmatron capabilities. Larger engines can be regenerated using multiple plasmatrons, or by using thermal management/non-uniform regeneration techniques.

It has been determined that the hydrogen rich gas will not spontaneously combust prior to reaching the soot trap under normal operating conditions of the engine. Thus, slow, uniform regeneration of the DPF could be achieved using both the thermal effect from the reformate as well as reducing capabilities and localized thermal effect of the hydrogen rich gas.

Experimental setup for determining the advantages of the hydrogen rich gas have been determined. Trap soot loading and regeneration tests will be carried out in the near future.

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