PREDICTIONS OF UREA DEPOSIT FORMATION WITH CFD USING AUTONOMOUS MESHING AND DETAILED UREA DECOMPOSITION

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MOTIVATION and BACKGROUND

- Urea-water solution (UWS) injection combined with Selective Catalytic Reduction (SCR) has developed as an effective method of meeting EPA and EURO NOx emissions regulations for diesel engines.
- One key challenge faced by modern urea/SCR systems is the formation of solid deposits of urea decomposition by-products that are difficult to remove.
- Urea deposits only form in a narrow range of wall temperatures and take many minutes to hours to form, which poses a challenge to conventional CFD tools.
- The autonomous CFD meshing code, CONVERGE, used in this study incorporates a detailed urea decomposition mechanism with Conjugate Heat Transfer (CHT) and spray-wall interaction models to predict wall temperatures with filming. The CFD code also takes advantage of a fixed flow approach and CHT super-cycling to dramatically accelerate the flow and spray simulation to reach the time scale required for appreciable deposit formation [1].
- The prediction approach is applied to a practical exhaust system urea deposit test bench published by Brack et al, 2016 [2].

CFD Geometry and Boundary Conditions

- A 12-step chemical kinetics [3,4] is adopted to model the urea decomposition and deposit formation.
- Compared to the classic molten solid urea decomposition model, where the urea thermolysis is modeled by a single chemical reaction, the urea detailed decomposition model itemizes each step during the urea thermolysis process and is able to predict reaction rate of various urea decomposition by-products (biuret, CYA, ammelide, etc.).
- The urea deposit formation only occurs within a narrow temperature range and is sensitive to temperature change.
- The Kuhnke splash model is used to model the spray/wall interaction. The Wruk heat transfer model is turned on for spray dry wall heat transfer prediction.

Fixed Flow Model and CHT Super-cycling

- For most aftertreatment cases, quasi-one-way coupling between exhaust flow and spray can be assumed.
- For a pulsed spray, the flow field can be frozen periodically. The solver stops solving the continuity, momentum and species equations when the flow is fixed. Only spray parcel tracking continues. The fixed flow model can speed up spray/edrainment film and deposition modeling substantially [5].
- Within each super-cycle of the wall CHT, the solver gathers the heat transfer coefficient data and calculates the wall temperature in a steady-state manner at the end of the cycle. This feature allows the wall to reach thermal equilibrium at a much faster pace without tuning the solid heat capacity.

Cooldown Simulation

- A cooldown simulation is conducted to account for the cooldown period in the experiments before retrieving the deposit sample.
- Urea deposit data is mapped in the cooldown simulation from the pre-cooldown run.
- Spray is turned off along with the inflow. Wall temperature is allowed to cool down exponentially to the room temperature. With a fixed CFL, the cooldown simulation can run extremely fast.

REFERENCES

Abstract

An aftertreatment system to treat exhaust gas from a diesel engine is provided. The aftertreatment system comprises a selective catalytic reduction catalyst on a diesel particulate filter (SCRF-F); a first reductant injector connected to an exhaust gas passage upstream of the SCRF-F; a downstream diesel oxidation catalyst (DOC) disposed downstream of the SCRF-F; a selective catalytic reduction catalyst (SCR) disposed downstream of the DOC; a second reductant injector coupled to an exhaust gas passage positioned between the downstream DOC and the SCR; and a controller to determine a desired particulate matter (PM) oxidation rate in the SCRF-F and a desired system NOx conversion.

Introduction

Selective catalytic reduction (SCR) technology has been used to reduce NOx emissions from heavy-duty engines. The ultra-low NOx emission standard for the heavy-duty diesel engine has been proposed by the California Air Resources Board (CARB). To meet the stringent regulatory NOx emission standards for heavy-duty diesel truck engines, an ultra-low aftertreatment system needs to be developed. For example, an aftertreatment system has been studied that includes a downstream diesel oxidation catalyst (DOC), a selective catalytic reduction catalyst on a diesel particulate filter (SCRF-F) and a selective catalyst reduction catalyst (SCR). The major factors that influence the performance of such aftertreatment system in terms of NOx reduction are catalyst aging in the SCRF-F, ash loading in the SCR-F, transport of the platinum group metals (PGM) from the upstream diesel oxidation catalyst (DOC) to the SCR-F and unfavorable NOx/NO2 ratio at the point of reductant injection can lead to reduction of the NOx, conversion of the downstream SCR and the system. Thus, there is need to improve the aftertreatment system such that the NOx emission standards can be met at various engine operating conditions such as cold start and hot conditions and the particulate matter (PM) oxidation rate in the SCRF-F also needs to be increased at various engine operating conditions.

Aftertreatment System Description

Figure 1 shows the proposed system consisting of DOC, SCRF-F, DOCx downstream SCR, AMOX and two urea injectors. For this system due to the addition of a second injector, the total urea flow rate is divided into components ANR1 and ANR2 which represents the ANR values at the two injectors. This system increases the NOx conversion and the PM oxidation rate over the SCR system alone by leveraging the control system which determines the ANR, and ANR, based on NOx conversion and PM oxidation rate targets. The downstream DOCx maintains a NOx/NO2 ratio of 0.4-0.5 at SCR inlet for all engine conditions. Figure 2 shows the increase in NOx/NO2 ratio at the SCRF-F due to the NOx oxidation reaction in the DOCx. The results of the downstream SCR performance is used to develop an optimum control strategy for the two urea injectors in the system resulting in high NOx conversion performance and high PM oxidation rate shown in Figure 3. The control system and results from Figure 2 and 3 are part of the research from [2][3][4].

Advantages of the System

The different embodiments and examples of the aftertreatment system for a diesel engine and the method to control or operate the aftertreatment system described herein provide several advantages over known solutions for improving PM oxidation rate and the system NOx conversion efficiency. For example, illustrative embodiments and examples described herein includes a DOC which is directly upstream of a SCR. 60 The inclusion of this DOC increases local NOx/NO2 ratio to optimum values (e.g., NOx/NO2 ratio of 0.5) at the downstream SCR, which leads to higher fast SCR reactions and thus greater than 99.5% system NOx conversion efficiency. The downstream SCR performance in this system is increased by 30-40% depending on engine operation conditions. Additionally, among other benefits, illustrative embodiments and examples described herein allow better control of inlet ANR, for the SCRF-F and ANR, for the SCR, which lead to accurate control of NH3 coverage fraction in both the SCRF-F and the SCR.

Figure 1. Aftertreatment system with SCRF-F, a downstream DOCx, SCR and two urea injectors

Figure 2. NOx/NO2 ratio vs ANR1 at engine condition C (SCRF-F+DOCx+SCR with 2 urea injectors)

Figure 3. NOx conversion efficiency, ANR, PM oxidation rate, SCR-NOx, and SCR-ANR. NH3 concentration vs ANR1 at engine condition C (SCRF-F+DOCx+SCR with 2 urea injectors)

Conclusions

The advantages of the SCRF-F+DOCx+SCR system components (2 injectors) are:

1) The proposed system has a 99.2 to 99.9% NOx conversion efficiency as for all the engine conditions
2) The proposed system has a 0.013 to 0.070 g/min PM oxidation rate as compared to 0.005 to 0.040 g/min for the SCRF-F alone for all the engine conditions
3) The SCR-F+DOCx+SCR system components enables 3-4 times higher PM oxidation rates as compared to the SCRF-F system when ANR = 0 which is used in engine conditions where a higher PM oxidation rate and 91-95% NOx conversion efficiency is desirable.
4) The tradeoff between PM oxidation rate and NOx conversion efficiency can be determined by the controller algorithm in the SCRF-F+DOCx+SCR system, which can operate over a limited range of ANR, (0.72+0.08) and ANR, (1.04+0.02) conditions without a loss in NOx conversion efficiency and PM oxidation rate.
5) Aftertreatment systems inline with this system without the DOC after the SCRF-F are being considered for light duty diesel applications by BMW [5], VW [8] and Eaton [7]

References

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Patent Claims

What is claimed is:

1. An aftertreatment system to treat exhaust gas from a diesel engine, comprising: a catalytic exhaust reduction catalyst on a diesel particulate filter (SCRF-F); a first reductant injector connected to an exhaust gas passage upstream of the SCRF-F; a downstream diesel oxidation catalyst (DOC) disposed downstream of the SCRF-F; a selective catalytic reduction catalyst (SCR), a downstream diesel oxidation catalyst (DOC) disposed downstream of the DOC; a second reductant injector coupled to an exhaust gas passage positioned between the downstream DOC and the SCR; a controller to determine a desired particulate matter (PM) oxidation rate in the SCRF-F and a desired system NOx conversion based on engine conditions, and to control a first reductant injector and a second reductant injector from the second reductant injector based on the desired PM oxidation rate in the SCRF-F and the desired system NOx conversion.

Figure 2. NOx/NO2 ratio vs ANR1 at engine condition C (SCRF-F+DOCx+SCR with 2 urea injectors)

Figure 3. NOx conversion efficiency, ANR, PM oxidation rate, SCR-NOx, and SCR-ANR. NH3 concentration vs ANR1 at engine condition C (SCRF-F+DOCx+SCR with 2 urea injectors)