

Concept, Loading and Calibration Effects on the Emission Performance of NG-TWC for HD Engines

Rafal Sala BOSMAL Automotive R&D Institute, Ltd

Kauko Kallinen and Alexander Chernyshev Dinex Finland Oy

Thomas Wolff Dinex Deutschland GmbH

Andreina Moreno Dinex Finland Oy

Citation: Sala, R., Kallinen, K., Chernyshev, A., Wolff, T. et al., "Concept, Loading and Calibration Effects on the Emission Performance of NG-TWC for HD Engines," SAE Technical Paper 2022-01-1013, 2022, doi:10.4271/2022-01-1013.

Received: 14 Apr 2022 Revised: 07 Jun 2022 Accepted: 07 Jun 2022

Abstract

he environmental impact of heavy-duty vehicles powered by natural gas is considered to be less harmful compared to Diesel vehicles. Consequently, the share of vehicles using either compressed natural gas (CNG) or liquified natural gas (LNG) is expected to increase in the coming years. Since most Euro VI compliant engines operate with stoichiometric air-fuel ratio, the aftertreatment system (ATS) requires efficient three-way catalyst. With ever increasing prices on platinum group metals (PGM) over the past few years, three-way catalysts products have been exposed to wild fluctuations in cost that have had great impact on their

affordability. Given that stoichiometric operation is the most widely used calibration of heavy-duty natural gas engines, the trade-off between efficiency, calibration and PGM cost must be constantly reset. This study focuses on the evolution and transition from bimetallic palladium-rhodium (Pd:Rh) concepts to trimetallic platinum-palladium-rhodium (Pt:Pd:Rh) three-way catalyst (TWC) concepts where a reduction in PGM loading through washcoat improvements and catalyst architecture supported by catalyst simulation software can be achieved, while keeping emissions at comparable or better levels and exploring the effects of different calibrations to the overall performance.

Introduction

uture developments in the automotive sector will be driven by a mix of technologies in which internal combustion engines (ICEs) will still have a role to play $[\underline{1}, \underline{2}, \underline{3}]$. In a pathway to carbon-neutral mobility, research dedicated to developing low-carbon and alternative fuels is also increasing. Natural gas (NG) and biogas represent one of the most concrete alternatives, and its use is increasingly promoted in transport, both for energy security and local air quality reasons [4,5]. The absence of long hydrocarbon chains and aromatics makes natural gas a cleaner fuel than gasoline or diesel and able to guarantee lower gaseous emissions [6,7]. The abatement of gaseous emissions resulting from the combustion of natural gas and biomethane is traditionally handled using three-way catalysts on engines operating stoichiometrically [8,9]. Particle Number (PN) emissions from NG ICEs do not usually require control by particle filters [10] to meet the most recent emission limits e.g. EURO VI. If an emissions control device is applied, associated robust on-board diagnostic methods must also be implemented [11,12]. The three-way catalysts are complex, in the sense that multiple simultaneous reactions take place over a narrow window of operating conditions [13]. From these, the oxidation of methane causes the added difficulty of taking place at higher temperatures [14,15] requiring the use of Pd, which is the most active precious metal to catalyze the reaction in large quantities. Given the sharp price increase precious metals have experienced in recent years [16], three-way catalysts are required to have flexibility in terms of formulation, loading and ratios to ensure cost impact is minimized and performance is preserved. In this work, we study the effect of PGM loading, ratio and calibration on the emission performance of a three-way catalyst for heavy-duty applications by means of experimental testing in the laboratory and on the engine bench, supported by catalyst simulations performed with Exothermia software.

Experimental

Test Methodology

The test methodologies employed during the study included: Synthetic gas bench testing of laboratory-sized TWC samples, emission performance of full-size prototype TWC samples by means of engine dyno testing and catalyst simulation software.

For a given engine calibration, reduction of PGM loading must be accompanied by PGM ratio adjustments to help compensate the overall reduction in PGM content.

The model generated in the course of this study can be used to make theoretical predictions of the behavior of modified samples during the WHTC on the same engine. This provides a powerful, cost-effective and reliable method to perform catalyst optimization and concept design.

Engine calibration plays a decisive role in the behavior of a TWC under WHTC conditions. For the studied samples, the best calibration is that where fuel cut-off events take place and help oxygenate the surface of the catalyst, though this is accompanied by an increase in NO_x emissions, it also decreases the CH_4 and NH_3 peaks, helping to keep a more balanced emission mix with respect to calibrations not featuring fuel cut-off.

The ECU 2 dataset used also had a wider lambda window, allowing for changes in TWC concept to have a less dramatic effect on emissions. i.e. Pd:Rh and Pt:Pd:Rh TWCs with very different loadings and ratios can keep emissions under the legal limits. With a more restricted lambda window, such as that of the ECU 1 dataset, a change from Pd:Rh to Pt:Pd:Rh with a simultaneous significant reduction in PGM loadings would be expected to perform very poorly.

References

- Reitz, R.D., Ogawa, H., Payri, R., Fansler, T. et al., "IJER Editorial: The Future of the Internal Combustion Engine," *International Journal of Engine Research* September 24 (2019). https://doi.org/10.1177/1468087419877990.
- 2. Kalghatgi, G., "Is It Really the End of Internal Combustion Engines and Petroleum in Transport?" *Applied Energy* (September 2018). https://doi.org/10.1016/j.apenergy.2018.05.076.
- 3. Leach, F., Kalghatgi, G., Stone, R., and Miles, P., "The Scope for Improving the Efficiency and Environmental Impact of Internal Combustion Engines," *Transportation Engineering* (June 2020). https://doi.org/10.1016/j.treng.2020.100005.
- Bae, C. and Kim, J., "Alternative Fuels for Internal Combustion Engines," *Proceedings of the Combustion Institute, Elsevier BV* (2017). https://doi.org/10.1016/j.proci.2016.09.009.
- Distaso, E., Amirante, R., Calò, G., De Palma, P. et al., "Evolution of Soot Particle Number, Mass and Size
 Distribution along the Exhaust Line of a Heavy-Duty Engine
 Fueled with Compressed Natural Gas," *Energies* 13, no. 15
 (2020): 3993. https://doi.org/10.3390/en13153993.
- Amirante, R., Distaso, E., Di Iorio, S., Sementa, P. et al., "Effects of Natural Gas Composition on Performance and Regulated, Greenhouse Gas and Particulate Emissions in Spark-Ignition Engines," *Energy Conversion and Management* (July 2017). https://doi.org/10.1016/j.enconman.2017.04.016.
- 7. McTaggart-Cowan, G.P., Rogak, S.N., Munshi, S.R., Hill, P.G. et al., "The Influence of Fuel Composition on a Heavy-

- Duty, Natural-Gas Direct-Injection Engine," *Fuel* (March 2010). https://doi.org/10.1016/j.fuel.2009.10.007.
- 8. Zhang, Q., Xu, Z., Li, M., and Shao, S., "Combustion and Emissions of a Euro VI Heavy-Duty Natural Gas Engine Using EGR and TWC," *Journal of Natural Gas Science and Engineering* 28 (January 2016). https://doi.org/10.1016/j.jngse.2015.12.015.
- 9. John, B., Heywood, Internal Combustion Engine Fundamentals, Chapter 11 (McGraw Hill, 1988), 655
- Kontses, A., Triantafyllopoulos, G., Ntziachristos, L., and Samaras, Z., "Particle Number (PN) Emissions from Gasoline, Diesel, LPG, CNG and Hybrid-Electric Light-Duty Vehicles Under Real-World Driving Conditions," Atmospheric Environment 222, no. 1 (February 2020): 117126. https://doi.org/10.1016/j.atmosenv.2019.117126.
- Kumar, P. and Makki, I., "Three-Way Catalyst Diagnostics and Prognostics Based on Support Vector Machines," SAE Technical Paper <u>2017-01-0975</u> (2017). <u>https://doi.org/10.4271/2017-01-0975</u>.
- Dadam, S.R., Van Nieuwstadt, M., Lehmen, A., Ravi, V.K. et al., "A Unique Application of Gasoline Particulate Filter Pressure Sensing Diagnostics," SAE International Journal of Passenger Cars-Mechanical Systems 14, no. 06-14-02-0007 (2021): 105-116. https://doi.org/10.4271/06-14-02-0007.
- 13. Zeng, F. and Hohn, K.L., "Modelling of Three-Way Catalytic Converter Performance with Exhaust Mixture from Natural Gas-Fueled Engines," *Applied Catalysis B: Environmental* 182 (March 2016): 570-579. https://doi.org/10.1016/japcatb.2015.10.004.
- 14. Gelin, P., "Complete Oxidation of Methane at Low temperature Over Noble Metal Based Catalysts: A Review," *Applied Catalysis B: Environmental* 39 (November 2002): 1-37, doi:10.1016/S0926-3373(02)00076-0.
- 15. Ferri, D., Elsener, M., Kröcher, O., "Methane Oxidation Over a Honeycomb Pd-only Three-Way Catalyst Under Static and Periodic Operation," *Applied Catalysis B: Environmental*, Vol 220, p 67-77, January 2018, https://doi.org/10.1016/japcatb.2017.07.070.
- 16. https://platinum.matthey.com
- 17. Aoki, Y., Sakagami, S., Kawai, M., Takanashi, N. et al., "Development of Advanced Zone Coated Three-Way Catalysts," SAE Technical Paper 2011-01-0296 (2011). https://doi.org/10.4271/2011-01-0296.
- Wang, C., Tan, J., Harle, G., and Gong, H., "Ammonia Formation over Pd/Rh Three-Way Catalysts During Lean to Rich Fluctuations: The Effect of Catalyst Ageing, Exhaust Temperature, Lambda and Duration in Rich Conditions," *Environmental Science and Technology* (October 2019), doi:10.1021/acs.est.9b03893.
- 19. Lou, D., Ren, Y., Li, X., Zhang, Y. et al., "Effect of Operation Conditions and TWC Parameters on Emission Characteristics of a Stoichiometric Natural Gas Engine," *Energies* 13 (2020): 4905, doi:10.3390/en13184905.
- Jiang, D., Khivantsev, K., and Wang, Y., "Low Temperature Methane Oxidation for Efficient Emission Control in Natural Gas Vehicles: Pd and Beyond," ACS Catal. 10 (2020): 14304-14314. https://dx.doi.org/10.1021/acscatal.0c03338.
- 21. Mejía-Centeno, I., Martínez-Hernández, A., and Fuentes, G.A., "Effect of Low-Sulfur Fuels Upon NH₃ and N₂O