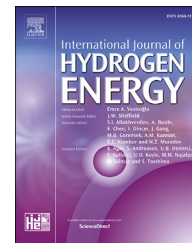




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Numerical model to analyze NO_x reduction by ammonia injection in diesel-hydrogen engines

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ABSTRACT

Nowadays, the even increasing stringent environmental legislations have promoted interest in alternative fuels for internal combustion engines. Particularly, hydrogen is becoming a promising fuel due to its high specific energy and low emissions production. Environmentally, the main disadvantage of hydrogen is the high level of nitrogen oxides (NO_x) which produces. In this regard, this work proposes a NO_x reduction method which consists on direct injection of ammonia (NH_3) into the combustion chamber. A numerical model validated with experimental measurements was carried out to analyze emissions and brake specific consumption in a commercial engine operating with diesel-hydrogen blends. Comparing to diesel operation, a 10% hydrogen content increases a 5.3% the peak pressure and 5.7% the maximum temperature. The CO_2 , CO and HC emissions are reduced but NO_x emissions increase up to 18.3%. Several injection instants and ammonia flow rates were analyzed, obtaining more than 70% NO_x reductions with a negligible effect on other emissions and brake specific consumption. It was found that the start of ammonia injection is too critical since the maximum NO_x reduction takes place when the temperature is around 1200 K. The NO_x reduction increases with the ammonia flow rate but an excessive quantity of ammonia can lead to un-reacted ammonia slip to the exhaust.

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Introduction

Internal combustion engines are widely employed in many sectors but they emit important levels of carbon dioxide (CO_2), particulate matter (PM), nitrogen oxides (NO_x), hydrocarbons (HC) and carbon monoxide (CO). Besides, these engines can also emit sulfur oxides (SO_x) depending on the sulfur content on the fuel [1]. For this reason, several international, national and regional legislations have been developed to limit these emission levels. In the recent years many technologies have been developed to reduce emissions, most of them unfortunately at the expense of reduction of efficiency. In this regard,

alternative fuels can provide both efficiency improvement and emissions reduction. Natural gas offers important advantages such as lower fuel cost and cleaner exhaust emissions. It has a high octane number, therefore, it is suitable for engines with high compression ratio, improving the efficiency significantly. Hydrogen (H_2) is another interesting alternative fuel which provides high thermal efficiency due to its high octane number, high specific energy, excellent flame speed, broad flammability range and low ignition energy requirement [2]. Besides, since hydrogen is carbon free, it leads to zero carbon based emissions such as CO_2 , CO and HC. A disadvantage is that the price of hydrogen is high.

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Hydrogen as a fuel is more suitable for spark ignition engines due to its high octane number [3–9]. In compression ignition engines, hydrogen is used under dual-fuel mode. The literature review indicates that the maximum hydrogen energy share in a dual fuel engine at high loads is limited from 6% to 25%, due mainly to higher in-cylinder peak pressure, knocking and high autoignition temperature [10–12]. The literature also indicates that environmentally the main disadvantage of hydrogen is the high NO_x emission levels, specially at high loads [13–16]. The reason is that the combustion temperature is increased with hydrogen addition and thus NO_x emissions, which are produced mainly at high temperatures. Many methods have been developed over the last few years to reduce NO_x emissions in hydrogen engines. Some of these methods, called primary measures, consist on reducing the amount of NO_x during combustion, for instance water addition [17–20], exhaust gas recirculation (EGR) [21–31], staged combustion [32], compression ratio reduction [33–35], modification of injection parameters [36–38], etc. Nevertheless, the increasingly restrictive legislation makes it very difficult to continue developing efficient primary measures at reasonable efficiencies. In this regard, other NO_x reduction methods, called secondary measures, remove NO_x from the exhaust gases by post-combustion cleaning techniques. The most employed secondary measures in engines are SNCR (selective non-catalytic reduction) and SCR (selective catalytic reduction). The former consists on reducing NO_x to nitrogen (N₂) using a nitrogen reducing agent such as ammonia, urea, cyanuric acid, hydrocarbons, etc. SNCR process has been successfully implemented in stationary power plants boilers and industrial furnaces. The main disadvantage of SNCR is that this is only efficient in a narrow temperature window centered at approximately 1200 K (±100), Jasminská et al. [39]. Flue gas from internal combustion engines does not reach this temperature, and reheating them reduces its efficiency. For this reason, catalysts are commonly employed to reduce NO_x from exhaust gas, what is called SCR. The main disadvantages of SCR are the poor durability and price. Besides, an additional space is required for the catalytic reactor.

Taking into account the disadvantages of SCR and the temperature requirements of SNCR, another option is to inject the reducing agent directly into the combustion chamber. Several researchers [40–44] verified that ammonia injection is more efficient than water injection because the latter decreases the combustion temperature. The capability of water to absorb heat of combustion reduces the temperature and thus the pressure, power and efficiency. Besides, a lower temperature promotes incomplete combustion and thus CO and HC emissions. Nevertheless, ammonia can reduce a higher amount of NO_x with a negligible effect on other pollutants and efficiency since ammonia performances as a fuel and does not reduce the combustion temperature [45].

The present work studies the possibility of injecting ammonia directly into the combustion chamber. The commercial engine MAN D2840LE V10 was analyzed. A numerical model was carried out to analyze its performance. After obtaining high NO_x emission levels using diesel-hydrogen

blends, ammonia was employed as NO_x reducing agent. More than 70% NO_x reduction was obtained with a negligible effect in brake specific consumption and emissions of other pollutants. Section [Computation of NO_x reduction by ammonia injection](#) describes the CFD model to reduce NO_x by ammonia injection and validation with experimental results. Section [Computation of the engine performance](#) describes the engine analyzed and the CFD model to analyze its cycle of operation, as well as the validation with experimental results. Section [NO_x reduction](#) combines the CFD models of Sections [Computation of NO_x reduction by ammonia injection](#) and [Computation of the engine performance](#) to analyze NO_x reduction in the engine using ammonia injection.

Computation of NO_x reduction by ammonia injection

chemical kinetics model

Among all NO_x components, almost 100% is NO. SNCR of NO using ammonia was first described by Lyon in 1975 [46]. Since then, the kinetics of the process was intensively studied. The first kinetic model was proposed by Miller and Bowman [47], based on 73 reactions and 19 species. Other models are those of Glarborg et al. [48], involving 104 reactions and 22 species; Miler and Glarborg [49], involving 134 reactions and 24 species; Skreiberg et al. [50], involving 191 reactions and 19 species, etc. Simplified models are also available in the literature, for instance those of Brouwer et al. [51] and Duo et al. [52], based on 2 reactions. The present work compared the models of Miller and Bowman [47], Glarborg et al. [48] and Miller and Glarborg [49].

CFD model

Given a set of m reactions which involve N species, Eq. (1), the local mass fraction of each species, f_k , can be expressed by Eq. (2), Versteeg and Malalasekera [53].

$$\sum_{k=1}^N \nu'_{kj} M_k \rightarrow \sum_{k=1}^N \nu''_{kj} M_k \quad j = 1, 2, \dots, m \quad (1)$$

$$\frac{\partial}{\partial t} (\rho f_k) + \frac{\partial}{\partial x_i} (\rho u_i f_k) = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{\sigma_\varepsilon} \frac{\partial f_k}{\partial x_i} \right) + \omega_k \quad (2)$$

In the equations above, ν'_{kj} are the stoichiometric coefficients of the reactant species M_k in the reaction j , ν''_{kj} the stoichiometric coefficients of the product species M_k in the reaction j , N the total number of species involved, ρ the density, μ_t the turbulent viscosity, σ_ε the turbulent Schmidt number and ω_k the net rate of production of the species k by chemical reaction, given by the molecular weight multiplied by the production rate of a species, Eq. (3).

$$\omega_k = MW_k \frac{dC_k}{dt} \quad (3)$$

where MW is the molecular weight and C the concentration. The net progress rate of reaction j is given by the production of the species M_k minus the destruction of the species M_k :

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