

Experimental-Numerical Analysis of Nitric Oxide Formation in Partially Stratified Charge (PSC) Natural Gas Engines

Stefano Cordiner, Giovanna de Simone and Vincenzo Mulone

University of Rome Tor Vergata

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ABSTRACT

Lean burn natural gas engines have high potential in terms of efficiency and NO_x emissions in comparison with stoichiometric natural gas engines, and much lower particulate emissions than diesel engines. They are a promising solution to meet the increasingly stringent exhaust emission targets for both light and heavy-duty engines.

Partially Stratified-Charge (PSC) is a novel concept which was conceived by prof. Evans (University of British Columbia, Vancouver). This technique allows to further limit pollutant emissions and improve efficiency of an otherwise standard spark-ignition engine fuelled by natural gas, operating with lean air-fuel ratio. The potential of the PSC technique lies in the control of load without throttling by further extending the lean flammability limit. It provides a relatively rich air-fuel mixture (fuel amount is less than 5% of the main charge) in the vicinity of the spark plug, while maintaining an ultra-lean homogeneous charge in the main combustion chamber area. A stable ignition kernel is then allowed to form in this region, to support the subsequent combustion process. The PSC technique does not require any modifications to the basic engine unless the adoption of a special spark-plug: this is one of its main advantages.

Since PSC is a relatively new technique, a thorough understanding of the physical processes involved is mandatory to guide the design process. To that aim, a joint experimental-numerical analysis has been performed in this paper, applied to a Ricardo Single Cylinder Research Engine equipped with the PSC spark-plug. Traditional homogeneous/stoichiometric and lean

PSC operating conditions have been compared in terms of performance and NO_x emissions, to finally put into evidence the coupling between PSC injection patterns and NO_x formation mechanism.

INTRODUCTION

Interest toward Natural Gas (NG) as a fuel for automotive applications is growing, prompted by several advantages. In fact, due to its wide flammability limits and very low knock tendency, it has extremely good combustion characteristics especially if used in high compression ratio engines, so leading to high thermal efficiency [1,2]. Moreover, due to the low carbon content, CO₂ emissions per unit energy [1] may be limited. These two favorable characteristics are ideal to reduce global CO₂ emissions, as European car manufacturers (ACEA) foresee the introduction of 120 g/km limit by 2012, continuing their reduction policy that got started from 186 g/km in 1995. Similar actions are implemented in Japan by JAMA and in Korea by KAMA [3,4,5].

Likewise, legislation is prescribing strong NO_x emission reduction (US 2010, for Heavy Duty (HD)) engines, and Euro VI limits, for passenger applications) [6,7].

Also in this case, NG is a promising fuel. To date, reduction of NO_x emissions are basically carried out by two strategies [8]:

- The use of stoichiometric mixtures, three-way catalysts and EGR (Exhaust Gas Recirculation), which led to very low emission;
- The use of lean-burn mixtures, to reduce flame temperature.

The latter strategy, as it may control load without throttle, would be optimal as high efficiency can be obtained.

An after-treatment device such as a three-way catalyst needs to be operated with a stoichiometric mixture. EGR, requires also a close-to-stoichiometric mixture to not meet misfire. The use of those strategies at the same time, allows safely NG-HD engines to comply with NO_x emissions according to US 2010 limits [9]. On the other hand, throttle is required to match the load with a consequent reduction of thermal efficiency at part load.

That disadvantage may be overcome by using lean-burn strategy. In fact, it allows to control load over a certain range by varying mixture composition (as for Diesel engines). Alternatively, lean-burn operation accompanied by an increase of compression ratio may also give similar advantages [2]. In this case, NO_x emissions in the order 1 g/kWh are obtainable only by ultra-leaning the mixture, i.e. for λ over 1.6 [10]. It is also cited in [10], that usual homogeneous operation in those conditions leads to go over Lean Misfire Limit (LML), and then engine stability is strongly affected as well as Total Hydro-Carbon (THC) emissions [11,12].

To extend the lean-limit of natural gas combustion, and improve efficiency and emissions, the Partially Stratified-Charge (PSC) technique [13] may be adopted [14,15,16,17]. The PSC technique allows to provide a relatively rich air-fuel mixture in the vicinity of the spark plug, while maintaining an ultra-lean homogeneous charge in the main combustion chamber area. This is achieved by injecting a small amount of natural gas, including less than 5% of the overall fuel mass, in the region of the spark plug just prior to ignition. Thus, the peculiarity of the PSC technique is the extension of the LML. Load may be controlled down to about two thirds of nominal load while also reducing NO_x more than with throttling partialization. Experimental investigations carried-out at UBC have shown that the use of PSC technique reduced NO_x by 30 per cent with respect to the lean homogeneous charge case, which was already a fraction of raw emissions given at part load by a stoichiometric-fuelled engine [18,10].

Since PSC natural gas is a new technology, a detailed understanding of the physical processes involved is mandatory to guide the design and optimization processes. To that aim, in last years, a numerical-experimental analysis on the combustion process that characterizes this approach, has been performed jointly by the University of Rome Tor Vergata and the University of British Columbia (UBC) Vancouver. Likewise, a detailed understanding of the physical processes involving pollutant formation is needed to better orient PSC engine design toward emission reduction.

In this paper, the analysis of a Ricardo Single Cylinder Research Engine equipped with the PSC spark-plug is performed by varying operating conditions. Nitric oxide

chemistry model is coupled with a RNG k- ϵ turbulence model and EDC turbulent combustion model (EDC).

EXPERIMENTAL SETUP

The experimental activities have been performed with a Ricardo Hydra Single-Cylinder Research Engine (SCRE) in the Department of Mechanical Engineering at UBC. The combustion chamber is a bowl-in-piston type with compression ratio of 9.25 and a squish ratio of 47.4%. General engine specifications are given in Table 1.

Table 1: Ricardo Hydra SCRE Configuration Geometry.

Number of valves	2
Firedeck geometry	Flat
Configuration	S.I.w/ PSC
Fuel	CNG
Bore $\times$ stroke [mm]	81.4 $\times$ 88.9
Connecting rod [mm]	158.0
Compression ratio	9.25:1
Displacement [cc]	463.0
Clearance volume [cc]	56.1
Inlet valve diameter [mm]	36.0
Exhaust valve diameter [mm]	33.5

Homogeneous fuelling was achieved by metering natural gas in the intake air upstream of the throttle body. The natural gas PSC charge is injected using a modified Bosch XR4CS spark plug, and injection is metered by an Omega SV121 solenoid valve, delivered through a capillary tube. Both the PSC spark plug and the implementation are presented in Figure 1 and Figure 2. The test engine was fully instrumented, including a piezoelectric pressure transducer for high-speed measurements of in-cylinder pressure and a comprehensive emission bench enabled measurement of exhaust levels of O₂, CO, CO₂, THC and NO_x.

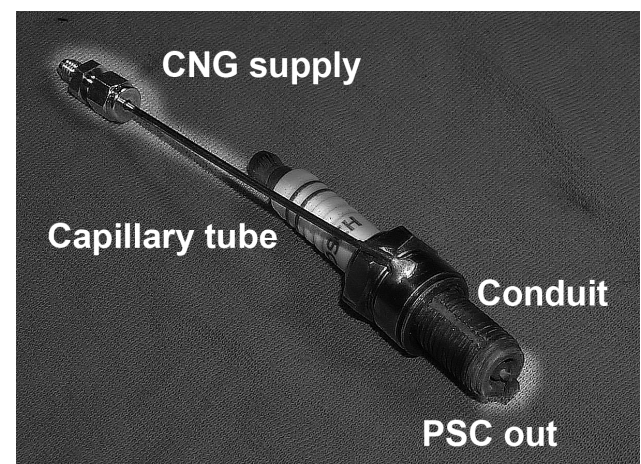


Figure 1: PSC spark plug injector.

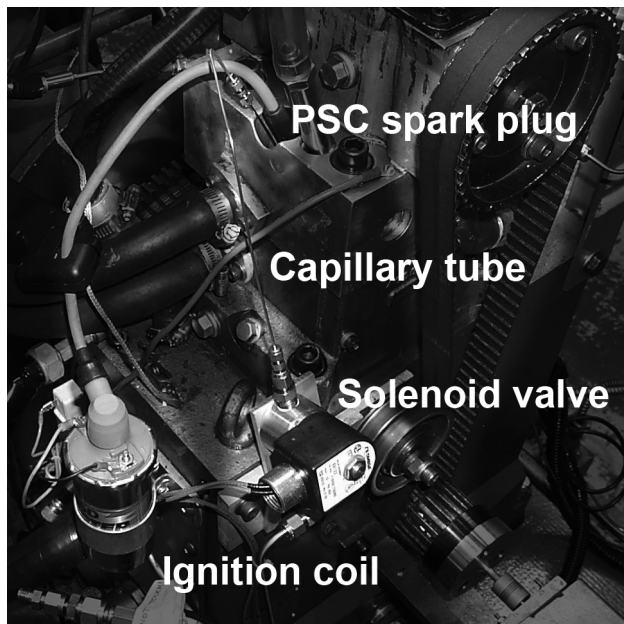


Figure 2: The Ricardo Hydra SCRE, and the PSC spark ignition system.

Testing of the SCRE was performed at wide open throttle (WOT) with an engine speed of 2000 RPM for homogeneous and PSC spark ignition. Engine load was varied by leaning-out the air fuel mixture [14].

Lean-burn operating conditions reduce the amount of NO_x in comparison with the stoichiometric case and much more if they are compared with the amount of NO_x obtained by throttling and keeping a stoichiometric mixture [14].

The advantages of the PSC technique are highlighted in Figure 3, where NO_x trend vs BMEP is reported with respect to different part-load management strategies. At 5 bar BMEP (63 per cent of full throttle load at 1500 r/min), NO_x can be reduced from 23 to 5 g/kWh by simply leaning-out A/F ratio. Partial stratification of lean charge cuts this value by a further 70 per cent, from 5 to approximately 1.5 g/kWh. It is also worth noting that 5 bar BMEP may not be reached at WOT without PSC. On the other hand, stoichiometric mixtures always keep high raw NO_x emissions as partial load is obtained with throttle control. It is also evident, by the data on NO_x reduction, that partial stratification does not introduce any “diesel-like” effects on NO_x. This may be due to the limited amount of A/F ratio variation over the combustion chamber, leading to a limited increase in pressure/temperature and oxygen availability.

However, to better understand the coupling between flow field, charge stratification patterns and temperature fields, a comprehensive 3D numerical model has been used whose details are given below.

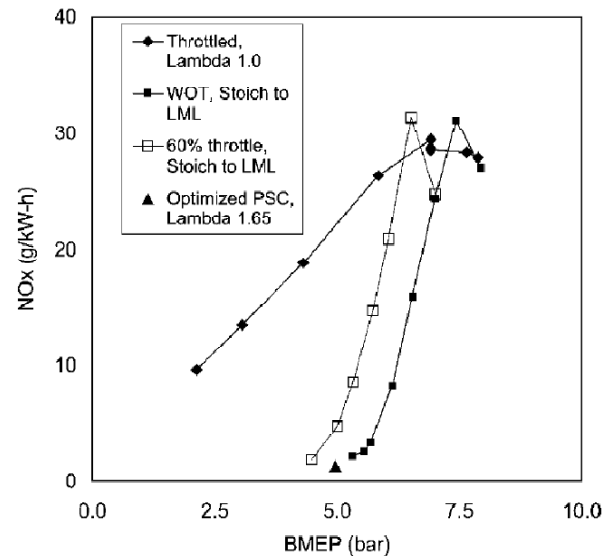


Figure 3: NO_x versus BMEP, comparing optimized PSC (BOI at - 70 CAD, 20 g/h) to throttled baseline and lean homogeneous baseline (1500 r/min, WOT and 60 percent throttle) [Errore. L'origine riferimento non è stata trovata.].

MODELING FRAMEWORK

GENERAL MODELLING ISSUES - The numerical code is characterized by a 3D approach. The computational domain includes intake and exhaust ports to take into account gas dynamic effects on volumetric efficiency. Boundary conditions are provided by means of a coupling to a 1D/0D engine code (FW 2001), already described in [16].

Ignition delay and kernel temperature by varying operating conditions are provided by a 1D ignition model getting as input data the instantaneous flow field and mixture composition in the vicinity of the spark-plug. RNG k- ϵ turbulence model and EDC (Eddy Dissipation Concept) combustion model are used to represent instantaneous flow field and combustion process evolution after ignition.

A kinetic mechanism for nitric oxide formation, the extended Zeldovich mechanism, has also been coupled with the ignition/combustion sub-models and used to predict NO formation.

IGNITION MODELING – The ignition process can be fundamentally described in terms of the breakdown, arc, glow-discharge phases [19,20]. The first two phases last no longer than a few microseconds together, and the gas in the path of the spark arc is initially ionized, and energy transfer takes place from the plasma to the surrounding gas. In the glow-discharge phase, the remaining electrical energy is “dumped” into the gas mixture, while the plasma expands through heat

conduction. At this point, the degree of gas ionization decreases sharply, resulting in a reduction in energy transfer efficiency. Typically, this ranges from 10% to 30% depending on the discharge method and local flow conditions [19].

The ignition process typically lasts approximately 1 ms. The final volume of the mature flame kernel is about 0.1% of cylinder volume at top dead center. Thus, ignition modeling can be decoupled from the main engine simulation, and can be treated as a 1D problem to improve computational efficiency with no major limitations [21].

Once activated, the 1D ignition code gets local flow and thermodynamic conditions as inputs, to determine the time at which the flame kernel reaches maturity as well as the expected burnt gas composition and temperature. Those results are then patched into the simulation at kernel maturity time, thus initiating the main combustion process.

The ignition process is represented by three separate but equally important models:

- kernel growth model
- plasma expansion speed model
- developing flame speed model

The ultimate objective is to derive a thermodynamically consistent model for spark ignition, taking into account energy transfer and phenomena in early combustion.

The presented kernel growth model follows the formulation of Tan and Reitz [22]. The flame kernel growth rate can be expressed as a sum of the plasma expansion speed and the developing flame speed

$$\dot{r}_k = \left(\frac{\rho_u}{\rho_k}\right) (S_{pl} + S_T) \quad (1)$$

where:

- $\dot{r}_k$ is kernel radius;
- ρ_u and ρ_k are unburned (bulk) and burned (kernel) mixture densities respectively;
- S_{pl} and S_T are the corresponding velocities for plasma expansion and developing flame.

Plasma expansion speed is dominated by heat conduction from the dissipating plasma to the surrounding fluid. Deshaies and Joulin [19] provided a closed-form expression for plasma expansion:

$$S_{pl} = \frac{\dot{Q}_{sp}}{A_k \left[\left(\frac{\rho_u}{\rho_k}\right) p + \rho_u (u_k - h_u) \right]} \quad (2)$$

where:

- $\dot{Q}_{sp}$ is the net energy transfer from the spark to the surround fluid
- A_k is the kernel surface area
- p is the kernel pressure, taken to be the same as the cylinder pressure
- u_k is the specific internal energy of the kernel, evaluated at the adiabatic flame temperature (T_{ad})
- h_u is the specific enthalpy of unburned gas.

The developing flame model is based on the work of Herweg and Maly [21]

$$\frac{S_T}{S_L} = I_o + (I_o)^{1/2} + \left(\frac{\|u\|_2}{\|u\|_2 + S_L}\right)^{1/2} \left[1 - \exp\left(-\frac{r_k}{L_e}\right)\right]^{1/2} \left[1 - \exp\left(-\frac{\|u\|_2 + S_L}{L_e} t\right)\right] \left(\frac{u'}{S_L}\right)^{5/6} \quad (3)$$

where:

- $\|u\|_2$ is the L_2 -norm of the instantaneous velocity
- u' is turbulent velocity fluctuation;
- L_e is the integral length scale representing the local turbulent flow field;
- S_L is the laminar flame speed in the vicinity of the spark region.

The laminar strain rate I_o , can be expressed as a linear combination of geometric and turbulence contributions:

$$I_o = 1 - \left(\frac{\delta_L}{15L_e}\right)^{1/2} \left(\frac{u'}{S_L}\right)^{3/2} - 2 \left(\frac{\delta_L}{r_k}\right) \left(\frac{\rho_u}{\rho_k}\right) \quad (4)$$

where δ_L is laminar flame thickness.

COMBUSTION MODELING - The Eddy Dissipation Concept (EDC) model by Magnussen [23,24] has been used throughout this work to model turbulent combustion. EDC, that is an evolution of the simpler EDM [25], relies on the assumption that combustion chemical reactions occur only at the smallest turbulent eddies. This means that chemical reactions in turn occurs only at the molecular scales (velocity u^* and length L^*) which are in the order of Kolmogorov scale [26]:

$$u^* = \left(\frac{c_{D2}^3}{3c_{D1}^2}\right)^{1/4} (\nu\varepsilon)^{1/4} \quad (5)$$

$$L^* = \frac{2}{3} \left(\frac{3c_{D2}^3}{c_{D1}^2}\right)^{1/4} \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} \quad (6)$$

Length and velocity scales are defined assuming that ε is calculated from a turbulence model (e.g. RNG k- ε), and that ε is invariant for all length scales according to the turbulence cascade hypothesis.

As mass ratio between the largest and smallest scales can be defined as follows:

$$\gamma^* = \left(\frac{u^*}{u'}\right)^3 = \left(\frac{3C_{D2}}{4C_{D1}^2}\right)^{1/4} \left(\frac{\nu\varepsilon}{\kappa^2}\right)^{3/4} \quad (7)$$

and that normalized mass transfer among the scales, can be defined as

$$\dot{m}^* = \frac{2u^*}{L^*} = \left(\frac{3}{C_{D2}}\right)^{1/2} \left(\frac{\varepsilon}{\nu}\right)^{1/2} \quad (8)$$

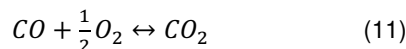
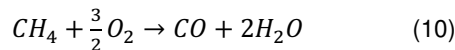
an expression for the mean rate of molecular mixing may be derived:

$$\dot{m} = \dot{m}^* \gamma^* = \frac{3}{4C_{D1}} \left(\frac{12C_{D2}}{C_{D1}^2}\right)^{1/2} \left(\frac{\nu\varepsilon}{\kappa^2}\right)^{1/4} \frac{\varepsilon}{\kappa} \quad (9)$$

Under the hypothesis that combustion is limited by molecular mixing, equation (9) can be used also to compute chemical reaction rates with the Eddy Dissipation Model (EDM) approach.

The addition, instead, of a given chemical reaction mechanism which processes a given mass rate according to equation (9), allows to get an extended turbulent combustion model where the series of the two processes is instead computed directly.

Methane chemical reactions are here modeled via the following two step reduced mechanism:



Chemical reaction rates have been computed by means of local constant pressure reactors, the reaction rate coefficients are given by the Arrhenius equation as outlined in Table 2.

Table 2: Arrhenius parameters for the two-step CH_4 combustion reactions.

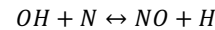
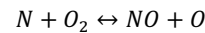
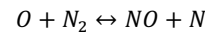
Reaction ^a	A [m ³ /mol·s]	n [-]	Ea [J/kmol]
$CH_4 + \frac{3}{2}O_2 \rightarrow CO + 2H_2O$	5.01e11	0	2.8e08
$CO + \frac{1}{2}O_2 \leftrightarrow CO_2$	2.24e12	0	1.7e08
^a $k_f = AT^n \exp(-E_a/RT)$ [m ³ /mol·s]			

The ISAT algorithm [26] has been used to accelerate chemical calculations (speed-up by two/three order of magnitude can be achieved).

As already stated, EDC and EDM models coincide as far as chemistry can be retained fast enough. However, in the context of this paper given the fact that combustion of lean mixtures is investigated, EDC has been utilized to have generally reliable combustion predictions even approaching very low turbulent combustion speeds.

NITRIC OXIDE CHEMISTRY MODEL - A kinetic mechanism for nitric oxide formation, the extended Zeldovich mechanism (thermal NO), has also been coupled with the ignition/combustion sub-models and used to predict NO formation [27,20,28].

Thermal NO is formed by oxidation of atmospheric nitrogen at relatively high temperatures in fuel-lean environment, and has a strong temperature-dependence. This process, described by the extended Zeldovich mechanism, consists of the following three main reactions:



Concentrations of oxygen and hydrogen radicals are calculated by partial-equilibrium considerations as follows:

$$[O] = kp_O [O_2]^{1/2}$$

$$[OH] = kp_{OH} [O_2]^{1/2} [H_2O]^{1/2}$$

while temperature and pressure are predicted locally by the 3D code. Calculation of NO rate and combustion process are decoupled as NO does not participate to heat release process (concentration is in the order of 1000 ppm). NO formation mechanism parameters are listed in Table 3.

Assuming a quasi steady-state for N, the overall rate for the three reversible, thermal NO reactions is given by:

$$\frac{d[NO]}{dt} = 2[O] \left\{ \frac{k_{f1}[N_2] - \frac{k_{r1}k_{r2}[NO]^2}{k_{f2}[O_2]}}{1 + \frac{k_{r1}[NO]}{k_{f2}[O_2] + k_{f3}[OH]}} \right\}$$