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Multi-zone thermodynamic modeling of combustion and emission formation in CNG engines using detailed chemical kinetics

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ABSTRACT

This study proposes an efficient and accurate methodology that combines detailed chemical kinetics with a validated multi-zone thermodynamic model to calculate the emissions of a spark-ignition, natural gas fueled engine. The relative air–fuel ratio has been changed from 0.8 to 1.53, and the nominal brake mean effective pressure has been varied from 0.2 MPa to 1.29 MPa.

The multi-zone model in-cylinder pressure and temperature traces, as well as other experimental engine quantities, have been considered as input data for the chemical submodel. The objective has been to reproduce and interpret the measured engine-out data in order to obtain insight into the in-chamber combustion and pollutant formation processes. The concentrations of nitric oxide, carbon monoxide, hydrogen, carbon dioxide and hydrocarbon, as well as the oxygen concentration after ignition, have been compared with experimental data and some of them have been compared with the results of conventional models.

The model results, based on detailed chemistry simulation, have been found to be in good agreement with experimental data for all the species at engine exhaust, and a higher prediction capability than that obtained through simplified reaction and chemical equilibrium methods has been shown. The influences of the uncertainties in RAFRs and unburned mass fractions on the calculated results are discussed. The unburned gas fraction, derived from the calculated and measured oxygen concentration at the engine exhaust, has been shown to be a way of correcting the hydrocarbon emissions.

1. Introduction

The emission performance of the internal combustion engine (ICE) is driven by more and more challenging regulations. Owing to the benefits of the “shale gas revolution” [1], natural gas (NG) has met an increasing diffusion in ICEs. It is utilized either in the form of compressed natural gas (CNG) or as liquefied natural gas (LNG). Compared to conventional fuels, NG combustion causes fewer hydrocarbons (HC) and CO_2 emissions, due to the chemical structure of the fuel and the absence of any evaporation phase [2]. The low carbon characteristics of the fuel are known to restrain the formation of benzene, and thus extremely low particulate matter (PM) levels are emitted. In spark ignition engines, NG can sustain higher compression ratios, owing to its high knocking resistance; as a consequence, higher thermal NO_x engine out emissions are generated, but a lower carbon monoxide (CO) fraction occurs at the engine exhaust [3–6]. However, the slower flame propagation speed requires an advance of the spark timing, and this reduces the port fuel injection engine performance [7].

A reliable diagnostic tool is essential for combustion and emission formation simulation in NG engines to assist experimental activities and support critical phenomena interpretation as well as new combustion concept analyses.

Models that simulate the combustion process in IC engines can be subdivided into single-zone models, multi-zone models and multi-dimensional models. The single-zone model is the simplest, since the in-cylinder temperature and composition are considered homogeneous (pure zero dimensional modeling). Thus, the performance of this model is not accurate enough to quantify peak temperature values and engine emissions. On the other hand, multi-dimensional models [8–10] usually couple a turbulence model (this can be either a RANS or a LES model) with a combustion model in order to simulate the flow and temperature fields in the cylinder during an engine cycle. However, these methods are cumbersome, even when standard RANS turbulence models are applied; furthermore, the chemical processes are calculated by means of a reduced reaction mechanism or by means of empirical laws.

Multi-zone based simulation codes are suitable for the diagnostics of existing engines, for performing parameter studies and for predicting optimum settings without resorting to complex multidimensional

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models [11]. In particular, multi-zone models are believed to be suitable for homogeneous charge compression ignition (HCCI) engines, since a subdivision of the chamber content into homogeneous zones is more realistic.

A two-zone combustion model, which couples an adiabatic core zone with a heat transfer model for the thermal boundary layer zone, was presented in [12] for HCCI engines. This model was later extended by adding a ring-pack zone (third zone) and was validated under turbocharged conditions, although no heat transfer between the core and other zones was considered [13]. A multi-zone combustion model, which included mass transfer between zones and implemented a reduced set of chemical reactions, was developed in [14] to assess the effects of mass transfer on the formation of HC and CO emissions. In [15], an "accelerated multi-zone model" that did not need to consider the heat transfer was developed. The methodology calculated the thermal stratification inside the cylinder on the basis of a computational fluid dynamics calculation for motored conditions. This model was benchmarked against coupled thermo-fluid dynamics and chemical kinetics calculations for a turbocharged (TC) gasoline HCCI engine and showed satisfactory agreement over a wide range of operating conditions, in terms of in-cylinder pressure and heat release rate predictions. Neshat [16–18] proposed a new multi-zone combustion tool that implemented an innovative heat transfer submodel and used not so detailed chemical kinetics mechanism to simulate the combustion process of n-heptane in an HCCI engine. This model contains a crevice zone, a boundary layer zone, some outer zones and a core zone. Heat and mass transfer between the zones are considered. The results are in line with experimental data pertaining to the prediction of in-cylinder pressure, NO_x, CO and UHC emissions.

Bissoli has recently developed a predictive multi-zone model for HCCI combustion [19], in which many factors that have a significant impact on combustion and emissions are taken into account: turbulence, heat and mass exchanges, crevices, residual burned gases, thermal and fuel stratification. The model improves the description of the mixture stratification phenomena by coupling a wall heat transfer model with a suitable turbulence model. A general overestimation of intermediate species is observed by comparing simulated with experimental data.

Unlike HCCI engine models, in which the mixture simultaneously ignites at multiple sites, the multi-zone model for conventional spark ignition (SI) engines needs to consider both ignition and flame propagation. Rakopoulos [20,21] and Asgari [22] developed a multi-zone model for the prediction of nitric oxide emissions in SI engines fueled with syngas and CNG, respectively. The super-extended Zeldovich mechanism [23,24], which considers six reactions, has been employed to calculate NO emissions [20–22], and the reaction rate model for CO prediction, which is described in [25] has been used. However, these NO and CO reaction mechanisms are simple and are isolated, and the predictions are very sensitive to some calibration constants that should be fitted to each engine working point.

In this paper, the combustion and emission formation processes of a spark-ignition (SI) CNG engine are analyzed with a multi-zone model that is coupled with a detailed chemical submodel for methane oxidation. The matching of an accurate multi-zone tool with a detailed chemical kinetics model represents a novelty in the literature on CNG engines. The calculated results have been compared with the experimental data as well as with the simulation results from previously developed thermodynamic models: the validation of the new model has in particular been carried out on different species at the engine exhaust (NO, CO, HC, O_2, CO_2, H_2 and CH_4). The objective has been to understand the role played by both thermodynamic modeling and chemical modeling in the simulation of combustion and emission formation in CNG engines.

Table 1
Main specifications of the TC engine.

Bore	70.4 mm
Stroke	78.8 mm
Compression ratio	10.10
Cylinder number	4
Displacement	1242 cm^3

2. Methodology

2.1. Experimental setup

The engine is a downsized turbocharged CNG engine for automotive applications [26]. The main geometrical specifications are given in Table 1. The engine has specifically been developed and optimized for CNG fueling, even though it also features bi-fuel capability. In fact, gasoline fueling, combined with a conservative spark timing strategy, is only limited to back-up operations in the case of a lack of CNG. The engine head features a disc-shape combustion chamber, two valves per cylinder and one side-located spark plug [27]. Furthermore, a wastegate valve, which allows selectable levels of turbocharging to be settled, controls the high-performance engine turbocharger. A Magneti Marelli, multipoint, sequential-injection module that features optimized calibration maps has been used.

The steady-state test cell is equipped with an eddy-current dynamometer that can adsorb a maximum power of 150 kW and a maximum torque of 300 Nm, and an encoder has been installed on the engine crankshaft to measure the engine speed. The engine has been instrumented with a hot-film air-mass sensor, which has been installed inside the intake system, two Coriolis mass-flow meters, installed in the fuel distribution pipes to measure both gasoline and CNG consumption, two air-fuel ratio universal exhaust gas oxygen (UEGO) sensors (one for rich mixtures and the other for lean mixtures), installed in the exhaust system, a pressure sensor, installed in the injection system rail, a hygrometer, installed in the intake system and thermocouples for measuring the temperatures of the intake flow, of the fuel and of the exhaust gases, and a water-cooled piezoelectric transducer, for taking accurate pressure time-histories within the combustion chamber. In addition, the bench is equipped with a multipurpose exhaust gas analyzer that can measure the THC (total hydrocarbons), MHC (methane hydrocarbons), NO, CO, CO_2, and O_2 levels in the exhaust gases of engines running on gasoline, diesel or alternative fuels (such as liquefied petroleum gas or CNG). All of the measured data are collected by a data acquisition system.

The accuracy of the measured flow-rates is 1.5% for CNG and 3% for air. The raw exhaust gas analyzers have a relative accuracy of 1% of the full-scale range, whereas span gases are provided with a 2% error of their nominal concentration.

2.2. Multi-zone model

The multi-zone model is based on the application of the first law of thermodynamics as well as of the perfect gas law to the combustion chamber content between inlet valve closing and exhaust valve opening. The diagnostic model requires the pressure time-history, measured in the SI engine cylinder, as a boundary condition. Fig. 1 reports a schematic of the engine where the combustion chamber volume is divided into an unburned gas zone (V_u) and a burned gas region (V_b), which here has been split into six 'zones' as an example. The numbers in the picture show each of the burned zones. In real simulations, a burned zone is generated each 5° crank angle (CA), and thus 15–20 burned zones (the exact number depends upon the combustion duration) are generally generated at the end of combustion (EOC). The following equation is obtained by constraining the sum of the volumes of the unburned region (V_u) and of the burned zones ($V_{b,i}$, where