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# 3D CFD simulation of a CI engine converted to SI natural gas operation using the G-equation

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Keywords: 3D CFD simulation G-equation RANS Spark-ignition Natural gas Re-entrant bowl	The conversion of heavy-duty CI engines to natural gas (NG) SI operation have the potential to increase the use of NG in the transportation sector in the United States. More, the increased turbulence of a bowl-in-piston combustion chamber can increase the flame speed under more efficient lean conditions. The main objective of this study was to investigate if a 3D G-equation-based RANS simulation (i.e., reasonable computational costs and running times) can predict the efficiency and emissions of such converted engine, for various NG compositions and operating conditions. The model was validated with experimental data from a single-cylinder CI research engine that replaced the fuel injector with a spark plug and fumigated NG inside the intake manifold using a low- pressure gas injector. Using a unique set of model tuning parameters, the model was able to qualitatively predict the effect of NG composition on engine performance and emissions over a range of operating conditions that changed spark timing, equivalence ratio, and engine speed. The model also captured the double-peak heat release rate seen at advanced spark timing in the experiments. The results showed that a lower methane number (MN) increased peak pressure and indicated mean effective pressure. Higher H/C ratio advanced combustion phasing. More, higher MN lowered nitrogen oxides but increased unburned hydrocarbons emissions. However, while a lower MN increased carbon monoxide (CO) production during the combustion process, there was no clear trend for engine-out CO emissions. Overall, the predicted gas composition sinvestigated here. However, the results suggest that the 3D CFD model described here is suitable for combustion phenomena analysis such the flame behavior in a bowl-in-piston combustion chamber.

### 1. Introduction

Forecasts predict that the internal combustion (IC) engine will continue to be the main power source in the transportation sector for the foreseeable future [1]. As a result, increased use of alternative fuels such as natural gas (NG) for on- and off-road vehicles can reduce the dependence on petroleum-based fuels and curtail engine-out emissions [2]. In addition to abundant resources in North America, NG's higher hydrogen-to-carbon (H/C) ratio reduces engine-out CO<sub>2</sub> emissions compared to conventional fuels, hence lower greenhouse gas emissions [3]

Conventional spark ignition (SI) engines can be easily retrofitted to NG operation [4]. The downside is a lower volumetric efficiency that decreases the engine power output compared to gasoline [5,6]. But NG SI engines can run leaner than their gasoline counterparts, which reduces the pumping work [7]. Furthermore, leaner operation not only decreases engine-out carbon monoxide (CO) and unburned hydrocarbon (HC) emissions, but also lowers nitrogen oxides (NO<sub>x</sub>) emissions

due to a lower combustion temperature [1,3,8,9]. Meanwhile, leaner operation increases the thermal efficiency by decreasing the heat transfer and increasing the combustion efficiency. The disadvantage of the lean combustion is a slower flame propagation speed, which can result in flame extinction before completely consuming the fuel-air mixture [7,10]. However, NG's higher octane-number compared to gasoline allows an increase in the engine compression ratio, which would increase both the flame speed and engine efficiency. This suggests that NG would be a good candidate to replace diesel in compression-ignition (CI) engines. But NG has a higher auto-ignition temperature compared to diesel fuel, which makes it difficult to control the engine operation without additional modifications [7]. A solution is for NG to only partially replace the diesel fuel, which will still initiate and control the combustion process [7]. However, this approach requires two fuel tanks and dual NG-diesel controls, which can greatly increase the engine cost [11]. Another solution is to convert the CI engine to SI operation by replacing the fuel injector with a spark plug that would ignite the fuel-air mixture [1,3,7,9]. NG is then fumigated inside the

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Nomenclature and Abbreviations		EVO	Exhaust Valve Opening
		IMEP	Indicated Mean Effective Pressure
AHRR	Apparent Heat Release Rate	IVC	Intake Valve Closing
ATDC	After Top Dead Center	MFB	Mass Fraction Burned
BTDC	Before Top Dead Center	RANS	Reynolds Averaged Navier-Stokes
CAx	CAD Corresponding to x % Mass Fraction Burned	SOC	Start of Combustion
CAD	Crank Angle Degree	ST	Spark Timing
DOC	Combustion Duration	TDC	Top Dead Center
DPIK	Discrete Particle Ignition Kernel		

intake manifold using a gas injector or injected directly inside the combustion chamber. The use of a hot surface is an alternative to using a spark plug (hence the name "hot ignition") for direct-injected NG engines, but it is not easily controllable at all operating conditions [7]. It is important to note that regardless of the retrofitting solution, appropriate engine calibrations are needed to control the high rate of pressure rise specific to premixed NG combustion and avoid knocking, especially at medium and high load conditions. This study investigates the more economical solution of replacing the fuel injector with a spark plug and the addition of a low-pressure gas injector in the intake manifold. This approach requires the least amount of engine modifications and/or calibrations, which is important for increased NG utilization. In addition, one of the cylinders can be used to compress the natural gas for applications that only have access to low-pressure NG gas lines (i.e., no access to CNG stations). However, the lack of information in the literature, particularly the information on the fundamentals of the combustion process in retrofitted single-fuel NG CI engines, can create difficulties in designing the controlling architecture for these engines.

Most of the literature that investigated fundamental NG combustion used experimental setups not representative of engine geometry (e.g., constant-volume vessels or rapid-compression machines) [1,9,12]. More, a major focus was on evaluating the efficiency of existing aftertreatment systems on the emissions of vehicles equipped with such retrofitted CI engines [13,14]. Further, numerous experimental investigations were focused on dual-fuel strategies, hence the large number of dual-fuel CFD simulations in the literature compared to CI engines converted to SI NG operation. Donateo et al. [15,16] built a model with suitable combustion chamber shape and engine control parameters from the database of different bowl-in-piston combustion chambers. This model then evaluated the performance and knocking tendency of DI engines converted to NG SI operation. Jiao et al. [17] and Yin et al. [18] used NG SI models to investigate the temperature and gas velocity distributions, and the overall turbulent kinetic energy inside bowl-in-piston chambers, which are different from the conventional roof-type combustion chamber in a gasoline engine. Adding to the combustion chamber geometry effects, NG composition varies with geographical source, time of year, and the treatments applied during production and/or transportation [3,7]. For example, in addition to (mostly) methane (CH<sub>4</sub>), NG also contains heavier hydrocarbons (ethane, propane, butane, etc.) and inert diluents (N<sub>2</sub> or CO<sub>2</sub>), which can significantly affect engine performance and emissions [19,20]. As a result, the engine control unit (ECU) must be capable of adjusting the engine operation to variations in NG composition [7]. All these issues suggest a need for both experimental and CFD work that not only investigate premixed combustion mode in a bowl-in-piston geometry (i.e., a diesel-like environment), but also the effects of NG detailed composition, if the economical retrofitting solution mentioned above is to be adopted.

The main objective of this study was to create a 3D numerical simulation of a heavy-duty CI engine converted to SI NG operation. The model was based on experimental data from a single-cylinder CI research engine that replaced the fuel injector with a spark plug and fumigated NG inside the intake manifold using a low-pressure gas injector. The goal was to build a tool capable of predicting the NG combustion behavior in a diesel environment (i.e., bowl-in-piston) that requires reasonable computational resources and/or running time. Of particular interest were predictions of NG composition effects on incylinder flame propagation and on the overall engine performance.

#### 2. Experimental setup

The experiments were conducted in a single-cylinder research engine (Ricardo/Cussons, U.K., Model Proteus), which is based on a commercial heavy-duty diesel engine (Volvo, Sweden, Model TD120). Table 1 shows engine specifications and Fig. 1 shows the engine setup. The original diesel injector was replaced by a NG spark plug (Stitt, USA, Model S-RSGN40XLBEX8.4-2) and NG was delivered using a gas injector (Rail Spa, Italy, Model IG7 Navajo, 3 seats). A piezo-electric pressure transducer (Kistler, Model 6011) was installed in the glow plug location and connected to a charge amplifier (Kistler, Model 5010) to measure in-cylinder pressure. An aftermarket engine management system (Megasquirt, Model 3X) controlled engine operation conditions such as gas injection, spark timing (ST) and duration. In-house-built data acquisition software (Scimitar) collected operating data such as engine speed, torque, air, coolant, and oil temperature, and air mass flow. Ref. [3] details the engine setup.

The engine oil and coolant temperatures were maintained constant throughout the experiments. Steady-state engine experiments were conducted at several operating conditions that changed ST from -10 to -30 CAD ATDC, equivalence ratio from 0.71 to 0.80 for methane and from 0.69 to 0.76 for natural gas, and engine speed from 900 rpm to 1300 rpm [3]. Table 2 details the gas chemical composition.

#### 3. 3D CFD simulation

Compared to a conventional SI engine (i.e., roof-type head), the combustion chamber geometry of the engine modeled in this work (i.e., bowl-in piston) changes the combustion behavior (i.e., the flame propagation) [9]. More, the experimental data (that will be discussed later) showed two heat-release peaks for advanced ST, which is not usually observed in conventional SI engines. As a result, a 3D CFD IC engine

Table 1
Engine specifications

Engine specifications.	
Engine manufacturer and model	Ricardo/Cussons, Proteus
Research engine type	Single-cylinder
Cycle	4-stroke SI PFI
Valves per cylinder	2
Bore [mm] x Stoke [mm]	$130.2 \times 150$
Displacement [liters]	1.997
Intake valve open	12 CAD BTDC exhaust
Intake valve close	140 CAD BTDC
	compression
Exhaust valve open	126 CAD ATDC
	compression
Exhaust valve close	10 CAD ATDC exhaust
Connecting rod length [mm]	275
Squish height [mm]	2
Geometric compression ratio	13.3:1
Combustion chamber	Bowl-in piston

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