



# Understanding the role of low reactivity fuel stratification in a dual fuel RCCI engine – A simulation study



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## HIGHLIGHTS

- Multi-zone, detailed chemical kinetics model used to assess natural gas stratification in RCCI.
- 5 heavy-duty engine operating points served as basis for simulation.
- Natural gas stratification is a promising strategy for partial load RCCI.
- Efficiency gain, THC/CH<sub>4</sub> emissions reduction, increased NO<sub>x</sub>.

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## ABSTRACT

Natural gas - diesel, Reactivity Controlled Compression Ignition (RCCI) is currently one of the most promising combustion strategies for the next generation heavy-duty engines. A major issue to be addressed for this dual fuel concept to become practically applicable is its low combustion efficiency and associated high methane emissions in partial engine loads. Introducing gaseous fuel stratification (by direct injection) is considered to be beneficial for combustion efficiency increase. Yet, the improvement potential of such natural gas stratification in RCCI engines is unknown. Modeling studies are needed to investigate this methane reduction measure because they can provide more insight to the combustion process than measurements alone.

The objective of this study is to assess the potential of RCCI with direct injected low reactivity fuel in terms of thermal efficiency and methane emissions. A broad range of measured, single point injected gas, operating points served as a basis for the simulation study. TNO's in-house, multi-zone, chemical kinetics based model was validated for those points and used to generate simulation results for different natural gas stratification profiles.

It is shown that gaseous fuel stratification in dual fuel RCCI helps to increase combustion efficiency and decrease methane and carbon monoxide emissions. At the same time, nitrogen oxides increase and (at some operating points) the emissions of non-methane hydrocarbons slightly increase too. The effect is strongest for the low load cases showing maximum improvement of combustion efficiency by 11 percentage point for in-extensive natural gas stratifications. The improvement potential reduces with increasing engine load. Thanks to the insights to the combustion process (given by the simulation results), explanations for the observed trends are provided, and important phenomena are identified that are associated with increased low reactivity fuel stratification.

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## 1. Introduction

Despite powertrain electrification and hybridization are rapidly progressing into the transport sector, it is expected that internal combustion engines will retain their position as the main propulsion technology for heavy-duty road transport and the maritime

sector. For decades, strict pollutant emission standards, and more recently, the targets for greenhouse gas (e.g. CO<sub>2</sub>) reduction, forces powertrain developers to seek for increasingly more sophisticated measures. Especially the push for CO<sub>2</sub> reduction strengthened the attention for advanced combustion concepts. The CO<sub>2</sub> benefit of applying advanced combustion concepts is due to the potential for higher thermal efficiency and use of alternative fuels, such as bio-fuels and natural gas (NG).

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## Nomenclature

### Abbreviations

aTDC	after top dead center
BMEP	break mean effective pressure [bar]
BR	blend ratio [%]
CA	crank angle
CFD	computational fluid dynamics
CH <sub>4</sub>	methane
CHR	cumulative heat released [J]
CN	cetane number
CO	carbon oxide
CO <sub>2</sub>	carbon dioxide
DF	dual fuel
DI	direct injection
EGR	exhaust gas recirculation
EVO	exhaust valve opening
FD	fuel distribution [-]
HC	hydrocarbons
HCCI	homogeneous charge compression ignition
HD	heavy-duty
HPDI	high pressure direct injection
HRR	heat release rate [J/CA]
IMEP	indicated mean effective pressure [bar]
IVC	intake valve closure
LHV	lower heating value [J/kg]
LTC	low temperature combustion
NG	natural gas
NMHC	non-methane hydrocarbons
NO <sub>x</sub>	nitrogen oxides
PCCI	premixed charge compression ignition
PM	particulate matter
PPR	peak pressure rise [bar/CA]

PRF	primary reference fuel
RCCI	reactivity controlled compression ignition
SOI	start of injection [CA]
SPI	single point injection (indirect to intake manifold)
TDC	top dead center
THC	total hydrocarbons
UHC	unburned hydrocarbons
$\Phi$	equivalence ratio [-]
$\dot{m}$	mass flow rate [kg/s]
CA10, CA50	crank angle at respectively 10% and 50% heat released
Ct	mixing coefficient [-]
dp/dCA	pressure rise rate [bar/CA]
N	engine rotational speed [rpm]
P	in cylinder pressure [bar]
T	temperature [K]
V <sub>disp</sub>	displacement volume [m <sup>3</sup> ]
Y	mass fraction [kg/kg]
$\gamma$	specific heat ratio [-]
$\eta$	efficiency [%]

### Subscripts

comb	combustion (efficiency)
d	diesel
g	gas
max	maximum
pump	pumping (efficiency)
res	residuals at EVO
wall	cylinder walls (losses)

Low temperature combustion (LTC) is a class of advanced compression ignition concepts that was extensively studied in the past decades. LTC strategies were proposed to reduce engine-out emissions of nitrogen oxides (NO<sub>x</sub>) and soot, while achieving higher thermal efficiencies than conventional diesel engines. Single fuel LTC strategies include homogeneous charge compression ignition (HCCI) and premixed charge compression ignition (PCCI), wherein the fuel is fully premixed and partially premixed, respectively. Those concepts were studied by many researchers, for example: [1–5] and proved to be inapplicable in practice due to the lack of control over the combustion process, leading to a limited load range and unstable operation [6].

Reactivity controlled compression ignition (RCCI) is a more recent LTC strategy in which two fuels are used to improve the controllability and load range compared to HCCI and PCCI, while retaining the vast advantage of high efficiency and low NO<sub>x</sub> and soot emissions at engine-out [7]. Various combinations of low and high reactivity fuels were used to demonstrate RCCI, amongst others: gasoline - diesel [8], ethanol - diesel [9,10], gasoline - biodiesel [11] and gasoline - (cetane number improved) gasoline [12].

Nowadays, natural gas (NG) attracts increasingly more attention as the low reactive fuel alternative in RCCI. NG is a so-called low carbon fuel which adds to the CO<sub>2</sub> emission reduction. Additionally, good availability, lower price compared to diesel and gasoline, and the potential to utilize renewable sources (e.g. biomethane) make the choice of NG in heavy-duty dual fuel RCCI engines attractive. NG-diesel RCCI is still relatively uncharted territory [13]. Most of the works covering this topic are still 3D CFD modeling studies [14,15] or single-cylinder research engine experiments [16–18]. Regarding applications in multi-cylinder, heavy-duty pro-

duction engines, TNO presented a NG-diesel dual fuel engine demonstrator working in RCCI mode, showing the possibility to reach 51% indicated thermal efficiency with ultralow NO<sub>x</sub> emissions [19]. Several challenges were identified in that study. A high engine-out CH<sub>4</sub> emission, especially at low loads, is the main drawback of NG-Diesel RCCI. Furthermore, variations of the input parameters result in high operation instability.

NG-diesel RCCI has challenging improvement points for the concept to become practically applicable. The most important ones are:

- further engine efficiency optimization,
- CH<sub>4</sub> emission reduction,
- increasing load range,
- combustion control to enable transient and robust operation under real-world conditions.

Various measures have been tested to improve the RCCI concept in general.

Proper NG-diesel blend ratio (BR) adjusting showed to be extremely important [20]. Lower BRs (low NG, high diesel) are used to assure better auto-ignition and lower CH<sub>4</sub> emissions at low loads [19,20]. This, on the other hand, leads to extensive wall impingement using early diesel injection strategies, therefore, resulting in increased non-methane hydrocarbon (NMHC) emissions. Higher loads enabled higher BR operation with increased thermal efficiency; BR of 96% was achieved with around 49% indicated efficiency [19]. Introducing uncooled Exhaust Gas Recirculation (EGR) combined with external heating of the intake air was identified as a promising measure to assure low load operation [19].

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