Increasing fuel flexibility and carbon efficiency of energy conversion in modern IC engines through advanced CAE technologies

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The on-going need to reduce exhaust gas CO_2 emissions to meet mandated legislation and energy concerns associated with the use of unsustainable oil-derivative fossil fuels is motivating the power generation, non-road and transportation sectors to find alternative technologies that will meet this targets. Thus far, incremental savings in CO_2 have been met through maintaining the established fuel infrastructure and focussing on enhanced fuel efficiency from the powertrain. However, achieving the required step change to "well-to-wheel" CO_2 emissions is far more challenging and requires an overhaul of the fuels being used as well as the modelling techniques used to design the new engines. Low carbon fuels can offer significant benefits over their conventional fuel equivalents, but their combustion characteristics and control strategies are not yet well understood.

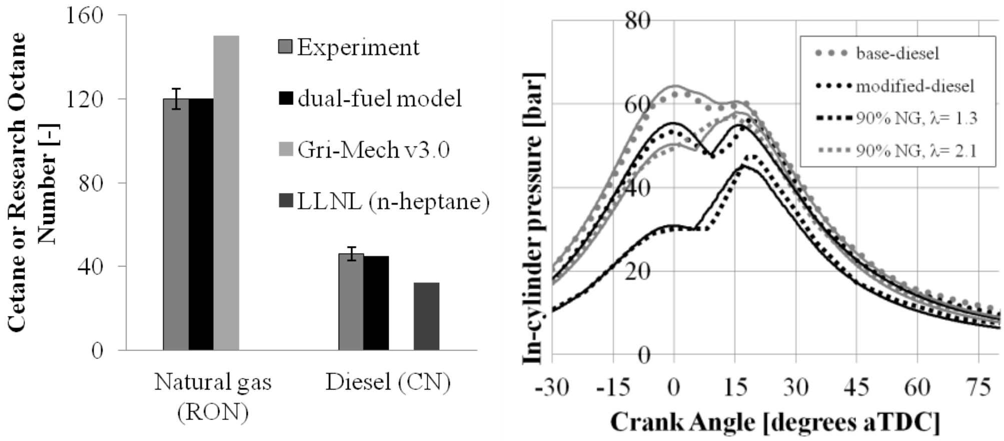

Figure 1 *Two examples of the validation tests performed for one of the developed fuel mechanisms. (Left) Virtual and measured Cetane and Research Octane Numbers of methane and diesel fuel surrogates. (Right) In-cylinder pressure vs crank angle at 2000 rpm 6.0 bar BMEP for four operating modes.*

Advanced Computer Aided Engineering (CAE) technologies which can account for key fuel characteristics are critical to bridging this gap and to reducing the R&D costs of re-optimising engine geometry, designing injection strategies, troubleshooting, etc. "Physics-based" CAE tools offer users a greater insight and can answer questions related to combustion phasing, combustion stability (ignition, misfire, flame propagation, knock, etc.), understanding sources of exhaust gas emissions (regulated and unregulated), characterising thermal efficiency (fuel efficiency, CO_2 emissions) and accounting for the interaction of

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fuels in dual-fuelled IC engines. Selecting the appropriate methods applied to simulate these aspects is of key importance.

This paper describes the state-of-the-art enabling simulation to facilitate the design of IC engine technologies for any fuel or any fuel blend. As part of this work, two new fuel models, one for fuel blends and one for dual fuel, have been developed using high-fidelity fuel-oxidation and emissions formation models and applied in advanced IC engine simulators to model fuel dependent processes such as ignition, misfire, flame propagation, knock etc.. These models can be used to meet the future demands of CAE and powertrain development in a multi-fuel forecourt.

Table 1 *Dual fuel engine operating points.*

	Base - diesel	**Modified-diesel**	**90% NG λ=2.1**	**90% NG λ=1.3**
Number of injections	3	1	1	1
EGR [%]	27	0	0	0
Natural gas substitution [%]	0	0	90	90
Intake composition, λ_{NG}	0.0	0.0	2.1	1.3
Throttle	-	-	no	yes

A demonstration of these methods is presented via the simulation of vast experimental databases of the most fundamental of engine/fuel metrics, the Research Octane and Cetane Number tests. A sample of the validation tests applied to the dual fuel model is shown in **Figure 1**. Next the model is applied to simulate a heavy duty dual-fuelled natural gas, diesel fuel ignited power generation application. **Table 1** summarises the engine operating modes that were simulated for the dual fuel case study. Results are presented in terms of combustion characteristics and emissions results.