Quasi-Dimensional Predictive Combustion Model Development for Spark-Ignited Methanol Engines

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Abstract **This article outlines the rationale, process, simulation results and future works for the development of a quasi-dimensional predictive combustion model specifically targeting large-bore heavy-duty engines operating with spark-ignition and 100% methanol.**

Keywords **Simulation, Spark-Ignition, Methanol**

I. Introduction

Methanol is a promising future marine fuel due to a lot of its advantageous properties. First, it is a liquid at ambient temperature and pressure, which saves a lot of storing and bunkering issues compared to a gaseous fuel. Second, methanol is one of the most widely traded and commonly shipped chemical commodities and is already available in abundance in more than 100 ports worldwide. Third, there are multiple sustainable production pathways. Last but not least, its molecular structure, high heat of evaporation, high flame speed plus the fact that it has no sulfur content render it low-emission and high-efficiency when combusted.

However, most of these advantageous properties in terms of combustion were proven on either light-duty SI engines or heavy-duty dual-fuel engines. As of today, test results of methanol SI operation in large-bore marine engines are still scarce so its potential remains largely unproven. Therefore, to enable a more comprehensive feasibility study, a robust predictive combustion model in a quasi-dimensional simulation environment will be extremely helpful to evaluate the true potential of such engines.

Quasi-dimensional combustion modelling means the combustion behaviour is predicted with zero-dimensional thermodynamics but the spatial variations such as piston movement, flame geometry, and cylinder geometry are also considered. Such an approach is a compromise between accuracy and computational effort, thus well-suited for performance evaluation. Vancoillie et al. has established a quasi-dimensional modelling methodology for light alcohol SI engines and validate it against test data on a light-duty engine [1]. This study will further examine its applicability to heavy-duty engines.

II. Methodology

A. Gas Exchange

To accurately estimate the combustion behavior inside the combustion chamber, it is important that the boundary of the combustion chamber, i.e., the intake and exhaust conditions are also well-captured.

This is taken care of by GT-Power, a commercial software package that solves the gas dynamics in the air-path with one-dimensional Navier-Stokes equations.

B. Combustion model

The core of the combustion model is the entrainment mechanism, Eqs. (1)-(2) proposed by Blizard and Keck [2],

$$\frac{dm_e}{dt} = \rho_u A_e (S_l + S_t) \tag{1}$$

$$\frac{dm_b}{dt} = \frac{(m_e - m_b)}{\tau} \tag{2}$$

Where S_l is the laminar flame speed; S_t is the turbulent flame speed; ρ_u is the density of the unburned zone; A_e is the surface area at the flame front, the subscript e denotes entrainment and τ is a time constant that can be associated to λ_T, the Taylor length scale, as in Eq. (3),

$$\tau = \frac{\lambda_T}{S_l} \tag{3}$$

Where λ_T can then be associated to Λ, the integral length scale; Re_t, the turbulent Reynolds number, and u', the turbulent intensity as defined in Eqs. (4) and (5)

$$\lambda_T = C_{TLS} \frac{\Lambda}{\sqrt{R_{e_t}}} \tag{4}$$

$$R_{e_t} = \frac{\rho_u u' \Lambda}{\mu_u} \tag{5}$$

C_{TLS} is the Taylor length scale multiplier that serves as a calibratable constant.

1) Laminar Flame Speed

Vancoillie et al. [3] calculated the laminar flame speed at different temperature, pressure, equivalence ratio and dilution ratio with a detailed chemical kinetic mechanism of methanol oxidation and established a correlation that is used in this study.

2) Turbulent Flame Speed

It was found [4] that the inclusion of thermodiffusive properties is key for turbulent flame speed estimation. In this study, Eq. (6) proposed by Gülder [5] is used due to its relative simplicity of implementation.

$$S_t = 0.6 C_{TFS} {u'}^{0.5} {S_l}^{0.5} {Re_t}^{0.25} \tag{6}$$

C_{TFS} is the turbulent flame speed multiplier that serves as a calibratable constant.

3) Flame Development

The transition from laminar flame to turbulent flame was found to be critical for premixed methanol combustion [6]. The flame development factor proposed by Dai et al. [7] as shown

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in Eq. (7) is used in this study to depict how this transition unfolds

$$\frac{S_{t,transient}}{S_t} = \left(\frac{r_f}{r_c}\right)^{\frac{1}{3}} \left(1 - e^{-\frac{r_f}{r_c}}\right) \qquad (7)$$

Where r_f is flame radius and r_c is a "critical" radius given by Eq. (8),

$$r_c = C_{FKG}\, \Lambda \qquad (8)$$

C_{FKG} is the flame kernel growth multiplier that serves as a calibratable constant.

C. *Test Data*

The dataset used to validate the proposed model is a high load IMEP sweep from a modified Scania D12 single cylinder research engine at KTH, the Royal Institute of Technology. The geometric information of the engine is listed in Table 1 and Figure 1 depicts the 25 operating points of the test. The measurement was done by varying boost pressures at a fixed engine speed 1200RPM. More detail about the engine and measurement equipment can be found in [8].

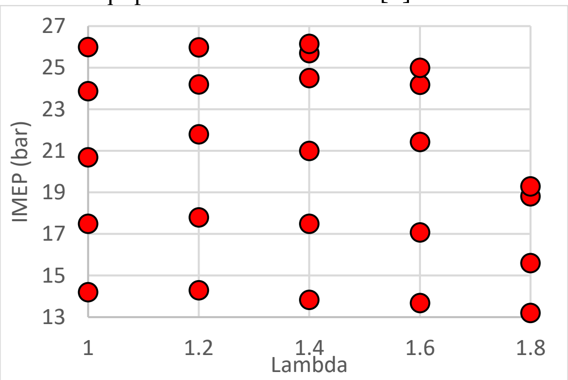

Figure 1. 25 operating points of the test.

Table 1 Geometric information of the Scania D12 engine.

Displaced volume	1950.8 cc
Stroke	154 mm
Bore	127 mm
Connecting Rod	255 mm
Number of Valves	4
Compression Ratio	12.7

D. *Calibration*

There are three calibratable multipliers, namely C_{TFS}, C_{TLS} and C_{FKG} in this study that are used as levers to fine tune the simulation outputs against the measurements. Optimization tasks were performed for each lambda to efficiently identify the optimal values of these multipliers that give the closest simulation results to the measurements. The resultant values of multipliers can be seen in Figure 2.

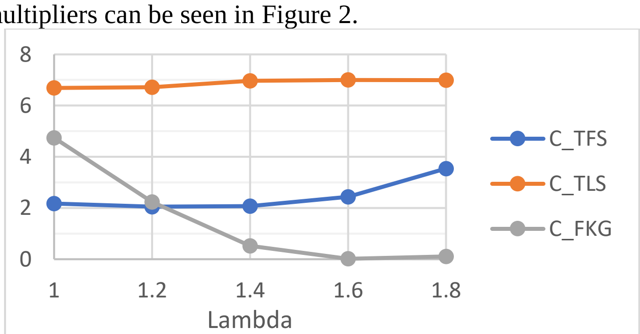

Figure 2 Optimized multipliers value for each lambda

III. Summary and Future Work

The root mean squared error (RMSE) between the measured and predicted indicated mean effective pressure (IMEP), crank angle at maximum cylinder pressure (CA@Pmax), crank angle at 50% fuel burned (CA50), 0% to 2% burn duration (CA02) and 10% to 90% burn duration (CA1090) were utilized as the performance indicators of the proposed model as plotted in Figure 3.

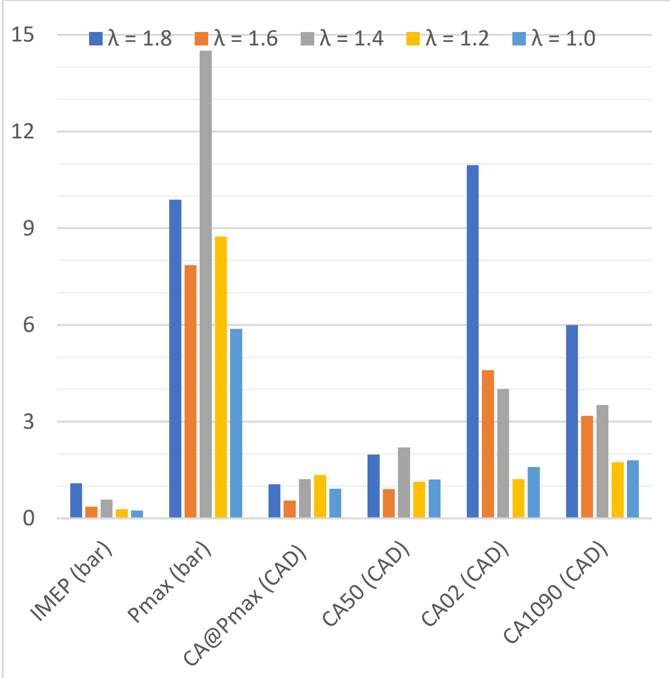

Figure 3. RMSE between the predictions and measurements

It can be seen that the proposed combustion model performed reasonably well when predicting IMEP and combustion phasing, but struggled in terms of combustion duration, especially when operating with higher lambda. Moreover, Pmax predictions are in general unacceptable. This may be due to the lack of laminar flame speed calculations above 100 bar in the correlation (it was evaluated at the cut-off of 100 bar at these conditions). This will be the subject of future work.

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