



A quasi-dimensional model for SI engines fueled with gasoline–alcohol blends: Knock modeling



L. Sileghem^{a,*}, T. Wallner^b, S. Verhelst^a

^a Department of Flow, Heat and Combustion Mechanics, Ghent University, Sint-Pietersnieuwstraat 41, B-9000 Ghent, Belgium

^b Argonne National Laboratory, Argonne, IL, USA

HIGHLIGHTS

- The aim of this study was to develop a knock model for alcohol–gasoline blends.
- A mixing rule for the ignition delay of alcohol–gasoline blends was proposed.
- Knock occurrence was experimentally investigated on a CFR engine.
- The proposed mixing rule and knock integral approach performed satisfactorily.

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ABSTRACT

As knock is one of the main factors limiting the efficiency of spark-ignition engines, the introduction of alcohol blends could help to mitigate knock concerns due to the elevated knock resistance of these blends. A model that can accurately predict their autoignition behavior would be of great value to engine designers. The current work aims to develop such a model for alcohol–gasoline blends. First, a mixing rule for the autoignition delay time of alcohol–gasoline blends is proposed. Subsequently, this mixing rule is used together with an autoignition delay time correlation of gasoline and an autoignition delay time correlation of methanol in a knock integral model that is implemented in a two-zone engine code. The predictive performance of the resulting model is validated through comparison against experimental measurements on a CFR engine for a range of gasoline–methanol blends.

The knock limited spark advance, the knock intensity, the knock onset crank angle and the value of the knock integral at the experimental knock onset have been simulated and compared to the experimental values derived from in-cylinder pressure measurements.

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1. Introduction

There is a renewed interest in methanol as alternative fuel for internal combustion engines. This has led to fleet trials of both high- and low-level methanol blends in China, Australia and Israel. China has declared coal-based methanol as a strategic transportation fuel to ensure its energy-independence. M85 vehicles have been around for some years, especially in coal-abundant provinces but now methanol is also finding its way into the densely populated coastal regions of China [1]. China's central government has launched a demonstration of light- and heavy-duty vehicles running on M85 (85% methanol and 15% gasoline) and M100 (100% methanol) in the Shanxi and Shaanxi provinces, as well as in the

city of Shanghai. In Israel and Australia, fleet trials with low-level methanol blends have also started [1].

Combustion knock is one of the major factors limiting the efficiency of spark ignition engines. It is caused by the autoigniting pockets of unburned gas [2]. The energy release associated with knock is usually very fast. This causes high local pressures and pressure waves across the combustion chamber. These waves can lead to mechanical and thermal damage to the engine.

As autoignition is a highly temperature and pressure dependent process, knock is often avoided by retarding spark timing, enriching the mixture, lowering the compression ratio or limiting the charge pressure in boosted engines. These classical measures usually reduce engine performance and efficiency. Alternative solutions may feature a combination of new technologies such as VVT (variable valve timing) or cooled EGR (exhaust gas recirculation) and fuels with elevated anti-knock resistance. In this respect, light alcohols, such as methanol and ethanol, are interesting

* Corresponding author.

E-mail address: Louis.Sileghem@UGent.be (L. Sileghem).

candidate fuels [3]. Alcohol fuels have a high knock tolerance for a variety of reasons. First and foremost methanol and ethanol have an elevated chemical resistance to autoignition, which is reflected in their high octane number (ON = 109) [4]. This is due to the single-stage autoignition behavior of alcohols. Compared to two-stage autoignition fuels such as gasoline, they do not exhibit a cool-flame reaction. This reaction takes place at temperatures below 900 K and promotes the main autoignition at high temperature. As autoignition in engines takes place at unburned mixture temperatures of 800–900 K, it is the prime reason for the reduced delay time of gasoline compared to alcohols [5]. Additionally the high latent heat of vaporization of light alcohols lowers the temperature of the unburned gas, further reducing the tendency to knock. In directly injected E85 engines the knock inhibiting effect of vaporization cooling has been shown to be comparable to the chemical effect [6]. For PFI (port fuel injected) engines, this effect is more modest. Finally, the increased (laminar) burning velocity of light alcohols helps to suppress knock as more end gas is burned before it can reach autoignition conditions [7,8].

As there is a renewed interest in alcohols as alternative fuel, an accurate predictive knock model for alcohols fuels would be of great value to engine designers.

The objective of this work is to develop such a model for (m)ethanol-gasoline blends using a simple mixing rule for the ignition delay of alcohol-gasoline blends. The model will be calibrated on pure gasoline (stoichiometric operation) and on pure methanol (stoichiometric operation) and with these two calibrations, the capability of the model to predict knock parameters of methanol-gasoline blends will be investigated.

2. Predictive knock modeling

Models to predict the autoignition of unburned mixture in spark-ignition engines range from simple empirical expressions to complex formulations featuring reduced or full chemical kinetics [9]. A widely employed empirical approach is to apply the conservation of delay principle proposed by Livengood and Wu [10]. According to this principle the overall ignition delay time can be found by integrating its instantaneous value during the compression and combustion stroke. This is analytically expressed by the knock integral reaching unity:

$$\int_{t_{IVC}}^{t_{KO}} \frac{dt}{\tau(t)} = 1 \quad (1)$$

where t_{IVC} and t_{KO} are the time at intake valve closure and knock onset respectively and $\tau(t)$ is the instantaneous autoignition delay time.

The autoignition delay time τ is the time during which a homogeneous mixture must be maintained at temperature T and pressure p before it autoignites.

The autoignition delay time τ at instantaneous cylinder pressure p , unburned mixture temperature T and composition is typically given by an Arrhenius expression representing the rate limiting step of autoignition:

$$\tau = Ap^n e^{\frac{B}{T}} \quad (2)$$

where A , n and B are parameters depending on the mixture composition (fuel, Φ , residual gas ratio). The most widely used parameter set for the ignition delay of spark ignition fuels was introduced in 1978 by Douaud and Eyzat based on recording the knock onset in a CFR engine for a range of running conditions and PRFs (primary reference fuels) with octane numbers between 80 and 100 [11].

Another way of calculating the ignition delay is with chemical kinetic models. The drawback for fuel blends is that the kinetic

models become very large and complex, with long calculation times as result, and that in many cases no models exist for blends of different fuels.

The Livengood–Wu integral gives an indication of when autoignition will occur in a completely homogeneous mixture. Completely homogeneous mixtures are unlikely in practice and autoignition will be triggered by ‘hot spots’ [12]. Thermal inhomogeneities caused by hot exhaust valves, turbulent transport during compression and large gradients of viscous stresses in boundary layers can cause these hot spots [12]. This means that autoignition can occur before the Livengood–Wu integral attains a value of unity. As a result, for two-zone thermodynamic engine models, such as the one used in this work, empirical expressions have been shown to yield performance no worse than comprehensive chemical kinetics schemes [9]. The inability of these models to reproduce local hot gas pockets and cyclic variation introduces uncertainties that outweigh those incurred by the simplified chemical kinetics. To consider these effects, multi-zone or 3D CFD approaches are necessary, employing either detailed chemistry or empirical expressions.

Still, the combination of two-zone modeling and the knock integral approach has been confirmed as a useful tool to estimate knock occurrence and intensity, which can be directly linked to the experimentally measured ratio of knocking to non-knocking cycles [13].

2.1. Autoignition correlation for gasoline

The combustion of many hydrocarbon species (gasoline included) exhibits two-stage ignition characteristics. This is especially true for most paraffinic hydrocarbons.

Autoignition correlations are often based on a simple, single-stage Arrhenius expression. These correlations lack detail regarding the cool-flame phenomena.

In the literature, two models were proposed to deal with the two-stage ignition characteristic, discussed below.

2.1.1. The model of Yates et al

Yates et al. [4,14] proposed an empirical model concept with a formfitting simplification of the overall ignition delay into four basic steps. These comprised (a) a pre-cool-flame delay at constant temperature, (b) an instantaneous cool-flame temperature increase (which could be zero), (c) a further delay at constant temperature, and (d) the terminal exothermic auto-ignition. It was assumed that this exothermic reaction sequence could be represented by a simple Arrhenius reaction formulation representing the gross, rate-limiting step, i.e.

$$\tau_h = \phi^{\beta_h} A_h p^{n_h} e^{\frac{E_h}{T}} \quad (3)$$

where the temperature profile exhibits a distinct step up at the cool-flame initiation point.

The calculation of the overall ignition delay needs to be undertaken in two stages by applying the conservation-of-delay principle proposed by Livengood and Wu, i.e.

$$\int_{t_0}^{t_1} \frac{dt}{\tau_{h,i}} + \int_{t_1}^{t_2} \frac{dt}{\tau_{h,CF}} = 1 \quad (4)$$

where t_1 is defined by the appearance of the cool flame and its associated temperature rise, and t_2 represents the overall ignition delay time. The autoignition delays, $\tau_{h,i}$ and $\tau_{h,CF}$ represent the characteristic exothermic reaction delay evaluated at the initial and post-cool-flame conditions respectively.

If the pressure and temperature are approximated as being constant during each stage, (and taking t_0 as zero), the integral simplifies to:

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