

Comparison and Sensitivity Analysis of Turbulent Flame Speed Closures in the RANS G-Equation Context for Two Distinct Engines

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ABSTRACT

Three-dimensional reactive computational fluid dynamics (CFD) plays a crucial role in IC engine development tasks complementing experimental efforts by providing improved understanding of the combustion process. A widely adopted combustion model in the engine community for (partially) premixed combustion is the G-Equation where the flame front is represented by an iso-level of an arbitrary scalar G . A convective-reactive equation for this iso-surface is solved, for which the turbulent flame speed S_T must be provided. In this study, the commonly used and well-established Damköhler approach is compared to a novel correlation, derived from an algebraic closure for the scalar dissipation of reaction progress as proposed by Kolla et al. [1]. The predictions from the two correlations are probed towards their sensitivities by means of experimental data from two distinctly different engine configurations: 1) a lean burn spark ignition natural gas engine for power generation, derived from a flat head/bowl-in piston compression ignition engine with roughly two liters of displacement per cylinder, and, 2) a small bore 250 cc single cylinder port fuel injected gasoline engine with a typical four-valve pent roof arrangement. The sensitivity of the flame speed closures towards the in-cylinder turbulent flow field is investigated for a sweep in turning speed for both engines close to full load. The numerical predictions in terms of pressure trace as well as heat release rates for both engines are compared to experimental test bench data and the predictive capabilities of the proposed closures for the two considerably different engine scales are studied. Additionally, the impact of two different RANS turbulence models (k - ϵ RNG and standard k - ω) on the results is discussed. The combustion regime is further classified in the Borghi diagram throughout the combustion event, where the flame speed closures are further investigated with emphasis on the early and late combustion stages.

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INTRODUCTION

Due to increasingly stringent emission regulations and the demand for higher efficiency internal combustion engines (ICE), much effort is devoted to the improvement of engine performance by means of combustion optimization. During the past decades, multidimensional models have been extensively developed towards engine applications.

As fields of velocities, turbulence quantities and scalars are available throughout the entire discretized domain, numerical results can complement data from optical diagnostics, which is often limited to small interrogation areas due to significant challenges as a consequence of the limited optical access in the confined time-varying geometry of IC engines (see e.g. [2]). The increasing

availability of computational resources in the past decades has enabled a transition from mean-cycle observations based on RANS modelling, towards large eddy resolving simulations (LES) allowing for computation of individual cycles. While this allows for investigation of single cycle phenomena such as knocking and cycle-to-cycle variations (CCV), LES of ICE engines is computationally extremely demanding if mean quantities are sought, since a statistically relevant number of cycles and phase-locked averaging is required. RANS, in combination with appropriate combustion models are therefore still widely used in the ICE development community since mean cycle quantities can be calculated very efficiently.

A wide range of length and time scales of flow and chemistry are present in turbulent combustion - many of which show considerable overlap [3] - especially throughout an engine due to the time-varying geometry leading to large changes in pressure, temperature and turbulence levels. As a consequence, a variety of models have been developed to tackle turbulent premixed combustion in the ICE context. These include, among others, the eddy break-up model [4], the Weller model [5] as well as the coherent flamelet models [6, 7]. Recently, a flamelet based combustion model in the ICE context employing a novel scalar dissipation rate (SDR) formulation was presented in [8] in a RANS framework. Among the available models, this work focuses on the G-Equation model, a level-set based flamelet combustion model. Following the initial derivation by Williams [9] for the laminar flame regime, the G-equation model was further extended by Peters [10] for the corrugated/thin flame regime. Its applicability in the RANS context has been demonstrated for fully premixed SI engines [11, 12] as well as partially premixed DISI engines [13, 14]. For the large engine used in this work and described more in detail below, a study focusing on the ignition using the G-Equation model has previously been reported in [15]. A multi-cycle analysis using LES and G-Equation for the small engine has been shown in [16].

As discussed in previous studies [12, 17], aside numerical issues concerning robust re-initialization of the G scalar field, the advancement of the level set representing the mean flame front hinges on a reliable correlation for the turbulent flame speed. A wide range of velocity and length ratios are further present in IC engine flows which need to be accounted for and hence numerous different correlations have emerged in the literature which correlate the turbulent flame speed to the laminar flame speed and turbulence quantities. One of the pioneering works in this field, and still widely used was presented by Damköhler [18], who's comparatively simple correlation assumes that the turbulent flame speed is solely related to the laminar flame speed and turbulence intensity, while the turbulent length scale and flame thickness are not considered. Despite these limitations, this simple model is widely employed in the IC engine community due to its robustness and simple implementation. In this study, the Damköhler closure has been adopted as a reference and compared to a more recently proposed correlation. Following Damköhler's early work, various turbulent flame speed correlations have been reported in the past decades, some of which include also dependence on the turbulent and chemical length scales, see e.g. [19, 20, 21, 22]. They are either based on the semi-empirical scaling law or constructed by passive scalar dynamics analysis. Recently, a new expression was proposed by Kolla et al. [1], which was derived by applying the Kolmogorov-Petrovskii-Piskunov (KPP) theory on the mean scalar dissipation rate algebraic closure and subsequently validated for different premixed flames across combustion regimes in [23]. The first application of this model to spark ignited IC engine combustion was recently presented in [24] where a turbocharged gasoline direct injection (GDI) engine was studied. Kolla's closure was found to capture the global combustion process well for low tumble ratio cases, but an underestimation at a higher tumble ratio was observed. Several possible reasons were identified and the authors conclude that further efforts are still required to reveal the root reasons. In this study, the predictive capabilities of this novel correlation is explored for two different engine sizes, running on two

different fuels (gasoline and natural gas) at stoichiometric and lean conditions, representing a considerable spread in length and time scale ratios. Variations in turning speed are examined for both engines at largely identical thermo-physical conditions to assess the impact of changing turbulence quantities and to explore the response of the two turbulent flame speed correlations hereto. In addition, two different turbulence models are compared to clarify the impact of changes in predicted turbulence quantities separately. No attempt has been made to compare the large number of turbulent flame speed correlations documented in the literature, as has been carried out e.g. in [25] using a Flame Surface Density combustion model in a LES context applied to a dump combustor with a sudden expansion as well as a triangular bluff body combustor. This paper starts from a description of the two engine experimental setups, the numerical method and respective settings applied followed by a discussion and concluding remarks.

EXPERIMENTAL SETUP

Liebherr Gas Engine (Large Engine)

The measurement concerning the Liebherr engine reported in this paper was conducted on an instrumented research engine version of the Liebherr G946 in-line six cylinders gas engine. The specification of the engine is listed in [Table 1](#). This engine will be denoted as "large engine" in the following.

Table 1. Liebherr lean burn gas major specifications

Displaced volume/cylinder	1991 cc
Stroke	150 mm
Bore	130 mm
Number of Valves	4

The research engine was fully instrumented, including six water cooled Kistler piezoelectric pressure transducers. The combustion data was recorded at a 0.1° CA resolution over 100 consecutive cycles. The average cycle was computed onwards together with the cylinder pressure standard deviation. Intake and exhaust temperatures and pressures were recorded at intake and exhaust manifold. Air mass flow was measured using a Sensyflow N200 sensor. Air-fuel ratio is calculated by taking into account the exhaust gas composition.

The engine is operated with a homogenous mixture of natural gas and air, which is guaranteed by the usage of a gas flow mixer. The related two engine operating conditions calculated in this work are at 1,500 rpm (50 Hz) and 1,800 rpm (60 Hz) respectively. Both operating points are close to the full load (BMEP = 16 bar).

SA 250 Engine (Small Engine)

Additional measurements and simulations have been carried out on a Swissauto Wenko 250 cc, port-fuel injected, single cylinder four-stroke spark ignition engine denoted as "small engine" in the following. The main specifications are summarized in [Table 2](#). The classical pent roof combustion chamber as well as intake and exhaust port are fully symmetric along a given plane through the cylinder center. The spark plug is located between the four valves. For each

operating point, 144 consecutive cycles have been recorder. The in-cylinder pressure is acquired by means of a piezo-electric pressure sensor (Kistler 6052) with a temporal resolution of 0.2° CA together with absolute values of the intake and exhaust pressures measured with Kistler 4075 and 4049 transducers, respectively. The temperature in the intake and exhaust is determined by radiation-protected thermocouples located at the same positions as the pressure transducers. The engine is connected to an APIcom FP75 eddy current brake.

The engine is fueled with a homogenous mixture using regular gasoline (RON 95) at stoichiometric conditions (lambda-controlled, Bosch LSU 4.9). For the simulations, the considered operating points are at 3,500 rpm and 4,000 rpm at 10.9 and 10.2 bar IMEP, respectively, which is close to full load.

Table 2. Major specifications of the investigated small engine

Displaced volume	250 cc
Stroke	56 mm
Bore	75 mm
Compression ratio	12.5:1
Number of Valves	4
Number of Cylinders	1
Fuel Injection	Port Fuel Injection (4 bar)

NUMERICAL METHOD

All the calculations performed in this study were conducted in an unsteady RANS (URANS) framework using the well-established flow field solver STAR-CD v4.24 [26] in conjunction with the es-ICE plugin for mesh motion [27]. In the following, turbulence and combustion modelling options are discussed, which are common to both engines investigated. Numerical settings, spatial discretization as well as initial and boundary conditions are discussed at the end of this section for the individual engines, since due to substantial differences in engine size and speed considerable discrepancies are present.

Turbulence Modeling

Two different eddy-viscosity based two-equation turbulence models were employed and compared in this work. The first one is the so-called Re-Normalization Group (RNG) variant of the k - ε model [28]. Due to its robustness and capability of accounting for flame-induced compression, expansion and rapid strain effect on the turbulence quantities, this model is widely used for ICE combustion simulation. Concerns have nonetheless been put forward regarding its appropriateness when applied to ICEs, in particular due to the k - ε model's shortcomings with respect to flow separation. This defect was pointed out by Kline et al. [29] when it was applied to many adverse pressure gradient flows and confirmed also in Rodi and Scheuerer's work [30]. Driven by these concerns, the authors have also tested the standard k - ω model [31, 32] coupled with the two-layer wall function in order to evaluate the model impact on the turbulence field prediction and its influence later on the combustion process. The reason to choose the k - ω is due to its ability to handle adverse pressure gradient and flow separation conditions as discussed e.g. in [32], which are present during valve opening. For the larger

engine considered featuring a flat cylinder head and high compression ratio, flow separation is also likely to occur due to high flow velocities from the squish into the bowl region as the piston approaches Top Dead Center (TDC).

Combustion Modeling

The G -equation combustion model was selected for this study which is a level-set flame front tracking technique. A field scalar G is introduced to indicate the flame front location, where an iso-surface defined by $G=0$ represents the flame front which separates the burnt ($G<0$) from the unburnt ($G>0$). Following Peters [10], the following transport equations for G and its variance G' , which is defined in equation (3), are calculated:

$$\frac{\partial}{\partial t}(\rho \tilde{G}) + \frac{\partial}{\partial x_i}(\rho u_i \tilde{G}) = \rho S_T |\nabla \tilde{G}| \quad (1)$$

$$\frac{\partial}{\partial t}(\rho G') + \frac{\partial}{\partial x_i}(\rho u_i G') = \rho S_T \frac{\nabla G' \cdot \nabla \tilde{G}}{|\nabla \tilde{G}|} + 2 \frac{\mu_t}{\sigma_i} \left[\frac{\partial \tilde{G}}{\partial x_i} \frac{\partial G'}{\partial x_i} \right] - C_s \rho \frac{\varepsilon}{k} G' \quad (2)$$

$$G' = G - \tilde{G} \quad (3)$$

The latter is required to reconstruct the turbulent flame brush thickness $l_{T,f}$ computed as:

$$l_{T,f} = \alpha \frac{\sqrt{G'}}{\tilde{G}} \quad (4)$$

where α denotes a model parameter for which unity is assumed here following [26].

For the turbulent flame speed S_T , appearing in the first term on the Right Hand Side (RHS) of equations (1) and (2), a closure is needed as will be discussed below. The second and third terms on the RHS of the equation (2) correspond to production of variance due to spatial gradients of G and dissipation, respectively.

The progress variable used for flame front cell sampling are defined in equation (5), where $Y_{f,u}$ represent fuel mass fraction at unburnt state and Y_f is the local fuel mass fraction.

$$C = \frac{Y_{f,u} - Y_f}{Y_{f,u}} \quad (5)$$

Laminar Flame Speed and Thermal Thickness Calculation

For the laminar flame speed, s_L , algebraic relations as proposed e.g. in [33, 34] are often used which correlate the laminar flame speed to unburnt temperature, pressure and air-fuel ratio. In the present study, unstrained laminar flame calculations have been performed instead, using the PREMIX package of CHEMKIN [35] to obtain the laminar flame speed and flame thermal thickness, δ_L^0 , defined as follows:

$$\delta_L^0 = \frac{T_{ad} - T_u}{\max(dT/dx)} \quad (6)$$

Surrogates are used to model the different fuels used in the two engines: For gasoline the iso-octane kinetics from [36] were adopted; for methane, the GRI-Mech. 3.0 [37] was used. The ranges of pressure, unburnt temperature and air-fuel ratios present in the two engines as well as the discretizations used for the pre-calculated table is given in Table 3. Linear interpolation is used when retrieving values from the table based on the local values in each CFD cell.

Table 3. Pressure, temperature and air/fuel ratio ranges used for the tabulation of the laminar flame speed (respective increments in parentheses)

Engine	Pressure [bar]	Temperature [K]	Air-fuel ratio [-]
SA250	5..80 (5)	300..1000 (50)	1.0
G946	20..150 (5)	700..1100 (50)	1.0..1.8 (0.05)

Turbulent Flame Speed Correlation

In the G equation context, modeling the turbulent flame speed constitutes the central task since it comprises all effects relating to turbulence-flame interaction. In the pioneering work of Damköhler [18] the following formulation was proposed:

$$S_T(\Phi) = S_L^0(\Phi) \left[1 + A \left(\frac{u'}{S_L^0(\Phi)} \right)^{\frac{5}{6}} \right] \quad (7)$$

It can be seen in equation (7) that for this closure the turbulent flame speed is only a function of the turbulent fluctuation speed u' and the laminar flame speed S_L^0 , related by an adjustable coefficient A which typically takes values of 3-4.

Aside the velocity scale ratio u'/S_L^0 , the closure recently proposed by Kolla additionally considers the length scale ratio l/δ_L^0 as well as further chemico-thermal contributions as presented in the following:

$$\frac{S_T}{S_L^0} = \sqrt{\frac{18C_\mu}{(2C_m - 1)\beta'}} \left[(2K_c^* - \tau C_4) \left(\frac{u' l_t}{S_L^0 \delta_L^0} \right) + \frac{2C_3}{3} \left(\frac{u'}{S_L^0} \right)^2 \right] \quad (8)$$

Where $C_\mu=0.09$ is a turbulence model constant and which is equal to the value used in the RNG k - ε and k - ω High Reynolds model, C_m is typically 0.7. The parameter β' accounts for curvature effects and here the default value of 6.7 is used. K_c^* represents the effects of dilatation rate. Turbulent-strain and scalar gradient interaction effects are included in the model parameters C_3 and C_4 and in equations (9) and (10):

$$C_3 = \frac{1.5\sqrt{Ka}}{1 + \sqrt{Ka}} \quad (9)$$

$$C_4 = 1.1(1 + Ka)^{-0.4} \quad (10)$$

which are both a function of the Karlovitz number defined as

$$Ka = \sqrt{\frac{1}{2(1+\tau)^{0.7}} \left(\frac{u'}{S_L^0} \right)^3 \left(\frac{l_t}{\delta_L^0} \right)} \quad (11)$$

with the heat release parameter τ :

$$\tau = \frac{T_{ad} - T_u}{T_u} \quad (12)$$

Validation of this model against lab-scale flame measurements over wide ranges of combustion regimes were reported in [23], with e.g. velocity scale ratios u'/S_L^0 spanning a range of 0 to 50.

At a first glance, Kolla's closure involves many parameters, but a detailed analysis, as provided in [23], shows that only u' , l_t and fuel type related parameters can be varied independently. In the original derivation [1], the turbulent integral length scale definition $l_t = u'^{1/3}/\varepsilon$ and laminar flame thermal thickness definition $\delta_L^0 = 2(1+\tau)^{0.7}\delta$, where δ is the Zeldovich thickness, were used to compute the length scale ratio. In this study, the integral length scale and thermal flame thickness are determined from equation (13) and (6), respectively, since pressure and temperature levels are changing throughout the engine cycle and cannot be determined beforehand as in the canonical configurations discussed in [23]. For the calculation of the integral length scale in the k - ω turbulence model, the dissipation rate ε is evaluated according to equation (14), as it is suggested by [26]. In view of the two different turbulence model formulations used here and the resulting different prediction of turbulence quantities as will be discussed below, and given the differences in the calculation of the integral length scale, an adjustable model constant f_{k0} has been introduced in the integral length scale formulation for the Kolla closure. This coefficient f_{k0} allows to cater for different predictions of the turbulent flow field, similar to the A coefficient in the Damköhler closure. No attempt has been made to change the shape and influence of C_3 and C_4 nor the other terms considered in equation (8), as each of them represents a physically sound derived contribution. The summary of the applied f_{k0} values can be found in Table 5 and Table 6.

$$l_t = f_{k0} C_\mu^{0.75} \frac{k^{1.5}}{\varepsilon} \quad (13)$$

$$\varepsilon = \omega \cdot C_\mu \cdot k \quad (14)$$

It can be observed in equation (8) that for $u'/S_L^0 \rightarrow 0$ the laminar burning speed is not recovered, as the molecular diffusivity has been excluded from the total diffusivity when performing the KPP analysis. This approach is justified, as the focus of the derivation for this closure was on turbulent flames with large Re numbers, as reported in [23]. No attempt has been made to introduce a modification to the formulation to address this (as proposed e.g. in [24]), since for the four operating conditions studied, vanishing levels



of turbulence intensity have not been encountered at the flame front where S_T is needed to displace the level set throughout the calculation, as will be discussed below.

Ignition Treatment

A simple energy deposition approach has been adopted here because, on one hand, the spark plug geometrical information as well as the exact orientation of the J-type electrode in the combustion chamber of the small engine were not available. The lack of local geometrical information may lead to inaccurate calculation of local flow and turbulence conditions, which are normally the inputs to advanced ignition models. On the other hand, the main objective of this work is to evaluate turbulent flame speed on distinct engines, while the ignition modeling is out of the research scope. The initial kernel radius was set to be the half of the electrodes gap.

Numerical Setup

Liebherr Gas Engine (Large Engine)

Due to asymmetric runner geometries, the full cylinder including intake and exhaust ports has been modeled, as it is shown in Figure 1.

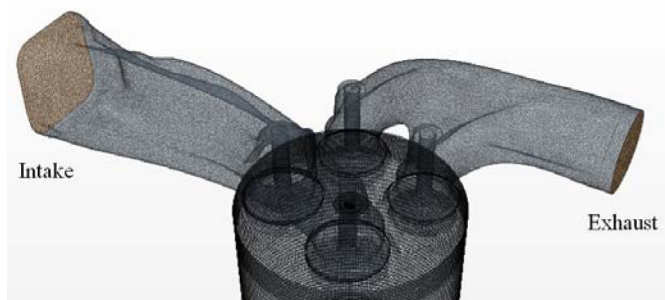


Figure 1. Computational domain of the Liebherr gas engine. Intake and exhaust ports are marked

The cylinder including the moving piston and valves uses a trimmed mesh and one prism layer was applied at the wall. An average cell size of 1.5 mm was used throughout the computational domain, which was reported to be sufficient in a former investigation [15]. The spark plug area was represented by a static mesh including the spark plug geometry. A cell refinement in the spark vicinity was also applied to resolve the small flame kernel following spark energy deposition.

The Pressure Implicit with Splitting of Operator (PISO) solver was chosen and the Monotone Advection and Reconstruction Scheme (MARS, for details cf. [26]) was used to discretize the momentum and turbulence equations. A baseline time step of 0.1° CA was used, while during combustion, intake and exhaust valve opening and closing this value is reduced to 0.05° CA to ensure numerical stability. Intake and exhaust pressure boundaries were derived by phase-locked averaging of 100 crank-angle resolved measurements.

Fixed wall temperatures were applied to the combustion dome, liner and piston crown region based on empirical values. The Angelberger wall function model was employed for the wall heat transfer calculation. For every engine operating point, two consecutive cycles were computed to minimize the impact of the estimated initialization. For the reference case, comparison of residuals for cycle 2 and 3 revealed differences of the order of 1 percent; in terms of peak cylinder pressure and peak HRR discrepancies of less than 0.3 percent were observed. A more detailed description of the model setup including also a grid sensitivity analysis can be found in [15].

SA 250 (Small Engine)

The specific numerical setup, aside the turbulence model, corresponds to the one used in the previous multi-cycle LES study presented in [16], where a more detailed description as well as a grid sensitivity study can be found. The time step was kept constant at 0.1° CA and is decreased during valve opening and closing by a factor of 5. The PISO algorithm is used for the coupling of pressure and velocity. The second order MARS scheme is used for the discretization of the momentum and turbulence equations. In order to save computational cost, only a half cylinder model of the SA 250cc single-cylinder engine is considered by making use of the symmetric engine design and introducing a symmetry boundary as indicated in Figure 2. Similar to the Liebherr engine, the intake and exhaust ports are meshed using a static polyhedral mesh, whereas the moving region, i.e. the combustion chamber and valves, are represented by a trimmed mesh. A prism layer of the size of 0.4 mm is imposed at the walls, whereas the average cell size corresponds to 1 mm. As the geometric features and orientation of the spark plug in the experiment are not known, the spark plug has been neglected in the computational grid.

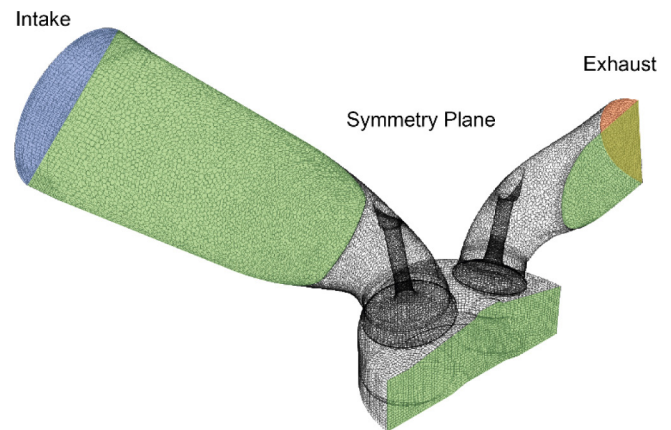


Figure 2. Computational domain of the SA 250 engine. Intake (blue) and exhaust (red) ports are marked as well as the symmetry plane (green).

At the intake and exhaust boundary, the phase-locked averaged pressure from the measurements is imposed. A homogeneous stoichiometric mixture of air and iso-octane (as a surrogate for gasoline) is prescribed at the intake. The Angelberger model is