

Influence of Binary CNG Substitute Composition on the Prediction of Burn Rate, Engine Knock and Cycle-to-Cycle Variations

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ABSTRACT

Since 0D/1D-simulations of natural gas spark ignition engines use model theories similar to gasoline engines, the impact of changing fuel characteristics needs to be taken into consideration in order to obtain results of higher quality. For this goal, this paper proposes some approaches that consider the influence of binary fuel mixtures such as methane with up to 40 mol-% of ethane, propane, n-butane or hydrogen on laminar flame speed and knock behavior. To quantify these influences, reaction kinetics calculations are carried out in a wide range of the engine operation conditions. Obtained results are used to update and extend existing sub-models. The model quality is validated by comparing measured burn rates with simulation results. The benefit of the new sub-models are utilized by predicting the influence the fuel takes on engine operating limits in terms of knocking and lean misfire limits, the latter being determined by using a cycle-to-cycle variation model.

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INTRODUCTION

Legal CO₂ emitting requirements and a worldwide increasing energy demand require a diversification on the fuel market, especially for automobile applications. When it comes to reaching the emission targets for passenger and freight transportation, natural and bio gases (CNG, Compressed Natural Gas and BNG, Bio Natural Gas) as well as synthetic methane based fuels (SNG, Synthetic Natural Gas) may play an important role. The advantages are well known compared to conventional fossil fuels: CO₂ savings of approximately 20 % can be realized compared to gasoline through a favorable H-to-C-ratio of methane. When adding renewable fuels, for example through electrolytically created hydrogen using excess solar power in daytime, the CO₂-benefit can be even stronger and reach almost 100 % when using biogenically generated methane.

Further CO₂ saving potentials lie in the improvement of the CNG engine efficiency. On the one hand, the high knock resistance of methane allows to run an efficiency optimized 50 % mass fraction burnt point (MFB50) and higher compression ratios. On the other hand, dethrottling can be achieved by using higher EGR rates, which are possible due to the wide ignition limits of methane. To benefit from these advantages, the 0D/1D-simulation represents an important tool that serves reliable results with little effort, especially for transient operations.

Based on the necessary simplification of the reality with 1D-models, 1D-simulations heavily depend on the quality of their used sub-models. For internal combustion engines it is of a high importance to model the combustion processes in great detail. Quasi-dimensional approaches, which are used to describe burn rates of natural-gas spark ignition engines, are mostly based on the modeling of the laminar flame speeds (s_L). However, direct measurements of laminar flame speeds are usually performed for an air-fuel equivalence ratio range between $\lambda = 0.7$ and 1.7 at pressures of only a few bar. Current approaches are extrapolated to unknown areas, which might cause contradictory data for laminar flame speed values.

To avoid problematic extrapolations for engine-related operation areas, reaction kinetics calculations are carried out to determine the laminar flame speed. The reaction mechanisms used for calculations follow known, physico-chemical principles which allow using a mechanism outside of its measurement-based validation range. Consequently, calculated laminar flame speeds can be approximated with a computing-time optimal correlation for 0D/1D-simulations.

When taking the influence of the fuel composition (for example rising amounts of hydrogen) on the laminar flame speed as well as knocking tendencies into account, the 0D/1D-simulation allows an even more detailed engine development process. In order to predict the operating range of lean running natural gas engines for example, determining knock and lean misfire limits is necessary. This becomes possible

when additionally using a cycle-to-cycle variation model. Hence, emission reduction potentials and improvements in fuel consumption of different engine setups can be investigated.

BURN RATE MODELING

The quasi-dimensional combustion model used in this study is presented in [1]. The laminar flame speed correlation proposed in this paper affects various equations regarding the combustion model. To clarify the influence, the principle idea of the combustion model will be outlined in the following.

Based on hemispheric flame propagation, the combustion chamber is divided into a burnt and an unburnt zone. Both zones are separated from each other by the flame front which is not considered as an additional, thermodynamical zone (see Figure 1).

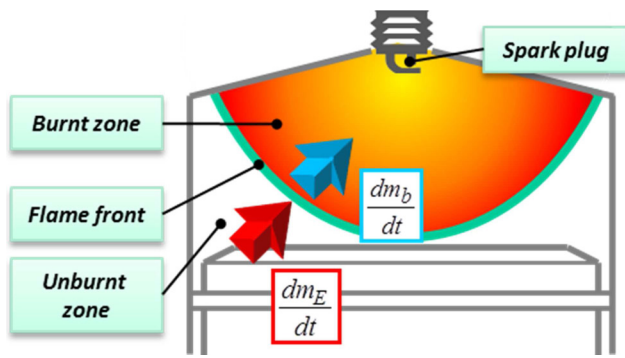


Figure 1. Schematic flame propagation [2]

The burn rate $\frac{dm_b}{dt}$ is calculated by means of the mass m_F entrained into the flame front and the characteristic burn-up time τ_L (Equation 1).

$$\frac{dm_b}{dt} = \frac{m_F}{\tau_L} = \frac{m_E - m_b}{\tau_L} \quad (1)$$

The characteristic burn-up time depends on the laminar flame speed s_L and the Taylor length l_T (Equation 2).

$$\tau_L = \frac{l_T}{s_L} \quad (2)$$

The laminar flame speed for gasoline is calculated in accordance with [3]. For methane, the calculation is based on *Glder* [4]. This calculation method extrapolates into unsurveyed ranges. Therefore, the laminar flame speed correlation proposed in this study substitutes the previous calculation method. Additionally, the influence of admixing ethane, propane, n-butane or hydrogen is implemented, enabling the calculation of binary CNG substitutes. The Taylor length can be computed with the global length scale l , the turbulence speed u_{turb} , the turbulent kinetic viscosity ν_T and the Taylor factor χ_{Taylor} with a value assumed to be 15 (Equation 3) [5].

$$l_T = \sqrt{\chi_{Taylor} \cdot \frac{\nu_T \cdot l}{u_{turb}}} \quad (3)$$

To calculate the turbulence speed u_{turb} , two different k- ϵ turbulence models can be used: a homogeneous, isotropic one as described in [5] and a quasi-dimensional model according to [6]. The latter model simplifies the tumble flow structure using a Taylor-Green eddy [7]. The resulting flow field yields the turbulence production using the same k- ϵ sub-models as are used in 3D-CFD but with simplified combustion chamber geometries. Thus, influences on the turbulent kinetic energy (TKE) such as changing cam durations and timings, as displayed in Figure 2, can be predicted. For combustion modeling, mainly the turbulence around top dead center firing (TDCF) is of great importance, where the model prediction matches the CFD simulation. Besides the influences on the Taylor length l_T and the characteristic burn-up time τ_L , respectively, u_{turb} also affects the entrainment velocity u_E (see Equation 4) which defines the entrainment mass flow dm_E into the flame front (see Equation 5). As a consequence, the consideration of TKE-influencing measures, besides reliable laminar flame speed models, is of importance in order to properly predict the engine operating range.

$$u_E = u_{turb} + s_L \quad (4)$$

$$\frac{dm_E}{dt} = \rho_{ub} \cdot A_{fl} \cdot u_E \quad (5)$$

The gas density in the unburnt zone (ρ_{ub}) is based on the corresponding mass and volume. The flame surface A_{fl} is calculated according to [1].

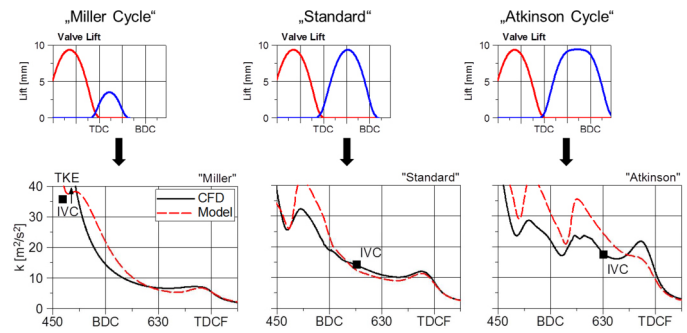


Figure 2. Predicted influence of cam duration on turbulent kinetic energy (TKE) [8]

LAMINAR FLAME SPEEDS OF BINARY, METHANE-BASED CNG SUBSTITUTES

To evaluate the quality of the hitherto used *Glder*-correlation [4], reaction kinetics calculations of laminar flame speeds are carried out for methane. Furthermore, s_L -changes due to admixing ethane, propane, n-butane or hydrogen cannot be considered in the engine simulation yet. In this chapter, these secondary fuel components are going to be investigated so that influences can be understood and applied in quasi-dimensional burn rate models.

Reaction Kinetics Calculations and Results

Reaction mechanisms are the basis of reaction kinetics calculations. Such mechanisms are developed for specific fuels and contain the equations of all (known) elementary reactions taking place during the combustion. These reactions are studied in detail for a wide range of boundary conditions to investigate on their temperature and pressure dependency as well as on their material properties such as mass transfer coefficients of all molecules that are listed in the reaction equations.

To perform reaction kinetics calculations, a software is needed to use the information stored in a reaction mechanism. In this study, Cantera [9] is used and controlled via the computer language Python. Cantera offers one-dimensional flames as a calculation scenario, which is used to determine laminar flame speeds. Furthermore, the reaction mechanism GRI-Mech 3.0 [10] is included. This mechanism has been developed and validated to calculate natural gases and is widely used for methane calculations. However, it contains only proprietary information about propane and n-butane chemistry [10]. Hence, the performance of other mechanisms was tested to capture this admixture influence by comparing calculation results with measured s_L values. For the admixture of propane, the USC C1-C3 mechanism [11] has been used. The USC C1-C4 [12] showed the best quality when calculating methane/n-butane mixtures.

It is important to note that with changing reaction mechanisms, the calculation results for pure methane diverge. As stated in [11], this divergence might result from the adaption of the USC mechanisms to represent higher hydrocarbons in addition to methane. To obtain consistent s_L -values for pure methane, the USC mechanisms have only been used to calculate the relative influence of admixing propane or n-butane. This relative influence has been applied to the absolute s_L values for pure methane, calculated with the GRI-Mech 3.0. Its results seem to be most trustworthy for pure methane in comparison with measurement data.

Via Python, it is possible to automate Cantera calculations over a wide range of boundary conditions. The boundary conditions used in this study are summarized in Table 1.

Table 1. Boundary conditions for reaction kinetics calculations

(Unburnt) Temperature (T)	300 – 1200 K
Pressure (p)	1-100 (-250) bar
Air-Fuel equivalence ratio (λ)	0.6-1.7(-flammability limit)
Residual exhaust gas (EGR)	0-50 mass-%
Secondary component (H_2 , C_2H_6 , C_3H_8 , n- C_4H_{10})	0-40 mol-%

The different ranges have been chosen to cover all possible engine operation conditions. The values in the brackets were calculated, but not again used, when applying the model approach to the results of the reaction kinetics calculations. They served as a validation basis for the model behavior outside of its adaption range. The blending rate limit of 40 mol-% results on the one hand from the non-linear

behavior of H_2 -admixture above 40 mol-%, where the transition from methane-controlled to hydrogen-controlled combustion begins [13]. On the other hand, a mixture of 60 mol-% methane and 40 mol-% hydrogen represents a methane number of 60, which already indicates a very high knocking tendency. Besides this, mixtures with considerably low methane numbers could be calculated by using high amounts of n-butane, for example 40 mol-% is equal to a methane number of 32.1.

Figure 3 shows the calculated laminar flame speeds of methane for varying residual exhaust gas fractions at different temperatures and pressures. While higher temperatures increase the speed of chemical reactions and, thus, the laminar flame speed, higher pressures or residual exhaust gas fractions show an inhibiting influence. Besides increasing the heat capacity, and thereby lowering the temperature, the residual exhaust gas dilutes the combustible mixture. This dilution decreases the fuel and the oxidizer concentration and, therefore, impedes the chemical reactions.

The pressure influence on the flame speed can be explained by *Le Chatelier's* principle [14]: High pressures promote reactions with fewer products than reactants. With a lower number of molecules, the pressure is reduced. For combustion reactions, this can be translated to the acceleration of chain-breaking reactions. In these reactions, fuel radicals recombine to a single stable molecule, hence breaking the chain reaction of the combustion and consequently decreasing the flame speed.

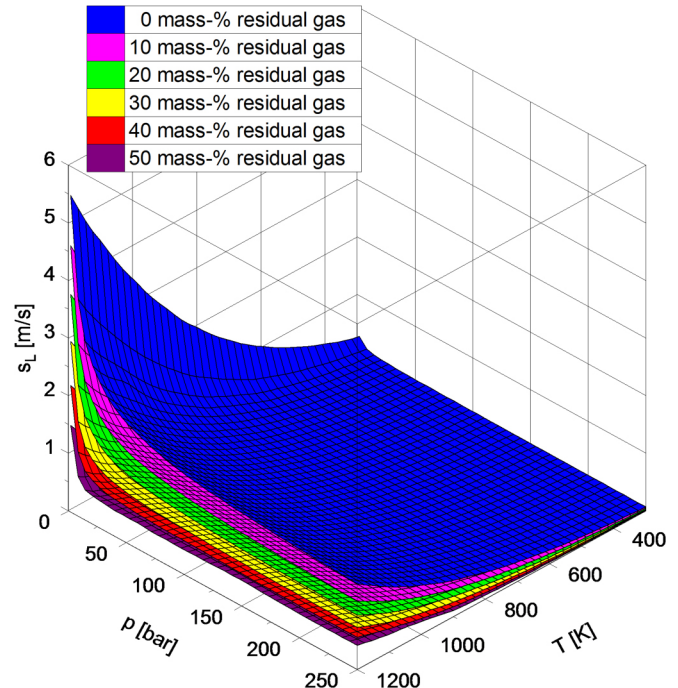


Figure 3. Residual gas, temperature and pressure influence on s_L of pure methane at $\lambda = 1$

The calculated influence of rising hydrogen amounts for different fuel-air equivalence ratios Φ ($=1/\lambda$) is compared with measurement data from [15] in Figure 4. With a higher amount of H_2 , the laminar flame speed of the mixture increases significantly due to the high reactivity of hydrogen molecules and matches the measured trend. For mixtures of methane with ethane, propane or n-butane, the same qualitative trends of calculation results can be observed. However, the absolute influence on the flame speed is less significant, which matches with the trends measured in [16]. On the contrary, the knocking tendency is strongly increased by adding even small amounts of n-butane to methane for example, as described in the later chapter "Fuel Composition Influence on Knock Simulation".

When varying Φ , a maximum in flame speed for slightly rich mixtures can be observed. This is a result of a chemical equilibrium, which only allows a conversion of all available oxygen with a surplus of fuel. With leaner or richer mixtures, the concentration of either reactant or oxidant decreases, which results in a lower speed of the combustion reactions. Additionally, the excessive amount of air or fuel has to be heated up, which brings a lower temperature and, thus, reduces the laminar flame speed.

It has to be noted that among other effects, laminar flame speed measurements might get influenced by flame wrinkling, for which a mathematical correction is necessary, eventually causing measurement uncertainties. Furthermore, flame wrinkling effects limit the range of available measurements to relatively low temperatures and pressures.

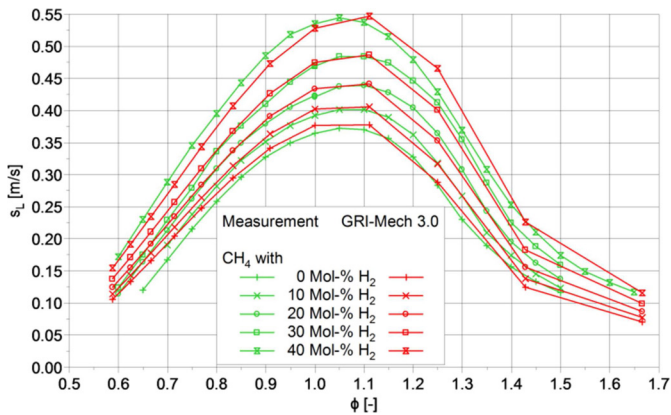


Figure 4. Comparison of measured [15] and calculated s_L -values with H_2 -admixture at 300 K and 1 bar

Figure 5 compares the influences of residual gas (EGR) and λ on s_L for pure methane at a pressure of 1 bar. The x-axes are scaled to match the curves of residual gas and λ for 300 K. The difference in the scale indicates the different influences of λ and EGR, since $\lambda = 1.3$ and a residual gas fraction of 22.1 mass-% represent the same degree of charge dilution. On the one hand, this results from different heat capacities of the air and the residual gas, which influence the heating of the unburnt gas as well as the flame temperature. On the

other hand, the different chemical behavior of the reactive excessive air at $\lambda = 1.3$ changes the reactions that take place during the combustion, compared to the nearly inert residual gas. The increasing difference between the blue and the red lines with higher temperatures represents the temperature dependency between λ and the residual gas influence, which needs to be taken into consideration when approximating the correlation for the laminar flame speeds.

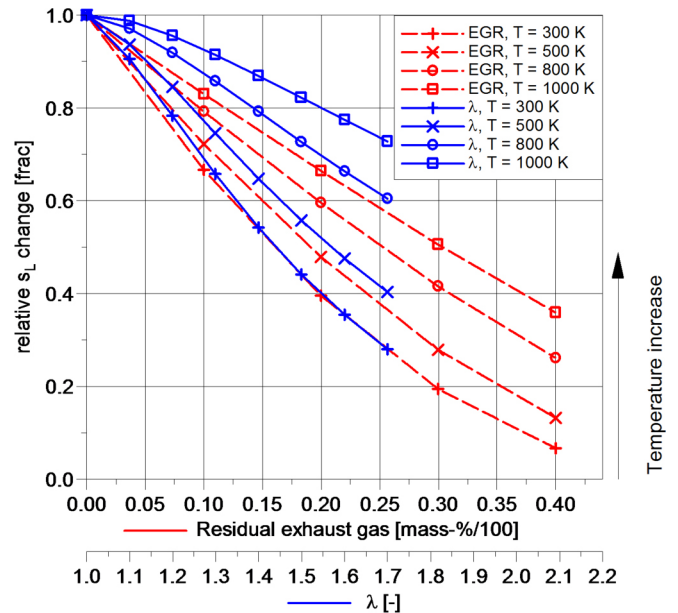


Figure 5. Comparison of λ and residual gas influence on s_L for CH_4 at $p = 1$ bar

In general, the calculated laminar flame speeds of all investigated mixtures show plausible trends over varied boundary conditions, matching available measurement data inside the range of measurement uncertainty. Since the single reactions that build a reaction mechanism can be studied in a far bigger boundary condition range than the laminar flame speeds, it is possible to use reaction mechanisms outside of their validation range [17]. Due to the lack of measurements, this range is relatively small. Therefore, only results of reaction kinetics calculation allow creating a laminar flame speed correlation for the engine application.

Model Approach

Figure 6 compares the laminar flame speeds that result from the Gülder-correlation [4], as described by the Equations 6 and 7, with reaction kinetics calculation results for pure methane at $\lambda = 1$.

$$s_L(\Phi, T, p, X_{EGR}) = s_{L,0}(\Phi) \cdot \left(\frac{T_u}{T_0}\right)^\alpha \cdot \left(\frac{p}{p_0}\right)^\beta \cdot (1 - f \cdot X_{EGR}) \quad (6)$$

$$s_{L,0}(\Phi) = 0.422 \cdot \Phi^{0.15} \cdot e^{-5.18 \cdot (\Phi - 1.075)^2} \quad (7)$$