

Two-Stage Ignition Occurrence in the End Gas and Modeling Its Influence on Engine Knock

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ABSTRACT

The most significant operation limit prohibiting the further reduction of the CO₂ emissions of gasoline engines is the occurrence of knock. Thus, being able to predict the incidence of this phenomenon is of vital importance for the engine process simulation - a tool widely used in the engine development. Common knock models in the 0D/1D simulation are based on the calculation of a pre-reaction state of the unburnt mixture (also called knock integral), which is a simplified approach for modeling the progress of the chemical reactions in the end gas where knock occurs. Simulations of thousands of knocking single working cycles with a model representing the Entrainment model's unburnt zone were performed using a detailed chemical reaction mechanism. The investigations showed that, at specific boundary conditions, the auto-ignition of the unburnt mixture resulting in knock happens in two stages. It is demonstrated that the commonly used knock integral is not capable of representing this behavior of the detailed chemical mechanism, meaning an improved approach for modeling the progress of the chemical reactions is needed for the calculation of the knock boundary. Based on these findings, a new two-stage knock integral approach capable of reproducing the auto-ignition behavior of the detailed chemical mechanism was developed. For this purpose, an enhanced three zone approach for modeling the influence of various parameters (pressure, temperature, exhaust gas fraction, air-fuel ratio, ethanol content and surrogate composition) on the ignition delay times of the mixture is proposed. Furthermore, a newly developed model for the ignition delay of the low-temperature ignition as a function of the boundary conditions is presented. Finally, the performance of the new two-stage approach is demonstrated and compared with the results achieved by the commonly used single-stage knock integral.

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INTRODUCTION

The ongoing trend of enforcing lower fuel consumption and tightening emission standards, combined with ever-increasing customer demands and severe competition on the global market is the main driving force for further improvement of the internal combustion engine regarding its efficiency and emissions. The most significant operation limit of spark ignition (SI) engines still prohibiting the accomplishment of these goals is the occurrence of knock, although this phenomenon has been observed for the first time almost 100 years ago. High compression ratios, which are desired for further improving efficiency, result in increased cylinder pressures and temperatures that, in turn, promote the occurrence of knock. The main theory behind this phenomenon is that detonation is being caused by auto-ignition and, thus, resulting in extremely rapid

heat release in the end gas ahead of the propagating turbulent flame. This causes very high cylinder pressures and temperatures that can potentially lead to total engine failure [1]. Thus, the auto-ignition phenomenon is a major obstacle in increasing the indicated engine efficiency [1, 2]. This is particularly important for turbocharged and downsized SI engines because of the higher inlet and, hence, cylinder pressures.

Nowadays 0D/1D simulations are being widely used in the engine development process. Thanks to the high prediction quality of the models and the low computational times, this is a powerful tool used to reduce development costs by partially eliminating the need for cost-intensive test bench investigations. The existing models for predicting knock in 0D/1D engine simulations however are

known for their poor performance and the great effort needed for their calibration. Hence, the reliable prediction of knock occurrence is a challenging task, especially if the entire engine map has to be considered.

GENERAL ENGINE KNOCK MODELING APPROACH

The 0D/1D knock models that have been developed in the past 50 years are generally based on the evaluation of an integral representing the pre-reaction state of the unburnt mixture (also known as knock integral, pre-reaction state integral and Livengood-Wu integral). Livengood and Wu originally formulated this correlation in 1955 [3]. They proved that the ignition delay time of an air-fuel mixture in motored and firing spark ignition engines can be estimated by evaluating an integral representing the degree of chemical reaction progress and thus the pre-reaction state of the mixture, [equation \(1\)](#).

$$1 = \int_{t=0}^{t=t_e} \frac{1}{\tau} dt \quad (1)$$

Hence, it is possible to predict when auto-ignition of a mixture in a firing engine will occur (end of integration t_e), if the ignition delay times τ are known at every integration step. These can be measured in a rapid compression machine or a shock tube. Subsequently, an Arrhenius-type equation, [equation \(2\)](#), can be calibrated by estimating the empirical constants C , C_1 and C_2 and then used for their calculation.

$$\tau \approx C \cdot p^{C_1} \cdot e^{C_2/T} \quad (2)$$

The integration process performed in [equation \(1\)](#) represents the process of concentration of chain carriers building up, until a pre-defined critical concentration has been reached and exceeded, resulting in an auto-ignition of the air-fuel mixture. The value of the pre-defined critical concentration is constant and thus independent of changes in the boundary conditions, such as e.g. an engine speed increase. The integration step in [equation \(1\)](#) should be chosen small enough, so that a constant speed of the chemical reactions during one integration step can be assumed (although it generally changes, as the mixture is being compressed and expanded in an engine).

Knock modeling approaches commonly used in the 0D/1D simulation today are all based on the correlation in [equation \(1\)](#). They evaluate the change in the pre-reaction state I_k of an air-fuel mixture between inlet valve close (IVC) or 90°CA before Firing Top Dead Center (FTDC) and knock onset (KO), as shown in [equation \(3\)](#) [16].

$$I_k = \frac{1}{n} \cdot \frac{1}{C} \int_{\alpha=\alpha_{IVC/90^\circ CA \text{ bFTDC}}}^{\alpha=\alpha_{KO}} \frac{1}{\tau} d\alpha \quad (3)$$

As soon as the pre-reaction state calculated in [equation \(3\)](#) exceeds a constant pre-defined value, the so-called critical pre-reaction state, knock onset has been reached. The $I_{k,crit}$ value at knock onset corresponds to the critical concentration of chain carriers in the original Livengood-Wu correlation that results in auto-ignition. Hence, it is obvious that the only difference between [equations \(1\)](#) and [\(3\)](#) is the integration domain and the ignition delay times needed for the integration process can be calculated with [equation \(2\)](#), after the empirical constants have been estimated. This is commonly done by fitting to measurement data. Generally, the mean values of the Entrainment model's unburnt zone parameters [4, 15] are used as knock model inputs.

Many different variations of the commonly used knock approach in [equation \(3\)](#) exist. By adding corresponding terms to [equation \(2\)](#), they consider the influence of various boundary conditions, such as the air-fuel equivalence ratio (AFR) and exhaust gas or Exhaust Gas Recirculation (EGR), on the ignition delay of the air-fuel mixture [17]. Such expansions of the commonly used knock modeling approach are generally based on measurement data. Alternatively, detailed kinetic reaction mechanisms for gasoline fuels that have been intensively developed in the recent years can be used to calculate the ignition delay times of air-fuel mixtures at various boundary conditions and hence to estimate the values of the empirical constants and to expand [equation \(2\)](#). This method has the main advantage of being able to cover a much wider range of boundary conditions than a parameter estimation performed with measurement data from a test bench. Of course, this is true only if the used kinetic reaction mechanism has been validated for all boundary condition variations of interest. Another significant advantage of the ignition delay estimation with detailed mechanisms is that no engine-specific effects affect the calculated values.

IN-CYLINDER REACTION KINETIC SIMULATIONS

Detailed kinetic reaction mechanisms cannot be integrated in 0D/1D simulations, as this would have a significant negative impact on the typically short computational times. Hence, a simplified approach reproducing the behavior of the chemical processes as accurately as possible is needed for modeling knock. In order to better understand how the chemistry behaves at in-cylinder conditions and to investigate the performance of the commonly used simplified chemistry approach - the knock integral, [equation \(3\)](#) - a simulation model representing the unburnt zone of the Entrainment model (or a small spot in it, as the model is scalable) was developed and implemented in Matlab/Cantera.

Simulation Model

Because of the complexity of detailed combustion kinetics of fuels, surrogate mixtures consisting of several hydrocarbon fuels are used in the gasoline reaction kinetics simulations [5]. A gasoline fuel with a Research Octane Number (RON) of 96.5 and approximately 10 vol. % ethanol content (E10) was chosen as a base fuel. The surrogate used in the present work is composed of iso-octane, n-heptane, toluene and ethanol. Thus, it accounts for the presence of ethanol in common gasoline fuels in Europe (up to 10 vol. %). The blending

rules are founded on the investigation findings in [6] that demonstrated the need for non-linear blending of iso-octane, n-heptane and toluene. Ethanol was blended linearly on molar basis as described in [7]. This resulted in a surrogate composition of 45.7% iso-octane, 13.6% n-heptane, 30.5% toluene and 10.3% ethanol (mass %) for the chosen base fuel. The reaction kinetics mechanism used in this work is a further development of the mechanism presented in [5] and consists of almost 500 different species.

The developed simulation model is based on an adiabatic reactor containing the surrogate-air-exhaust gas mass, Figure 1. In addition, a moving wall was installed to compress and expand the mixture and hence reproduce the piston movement. Furthermore, the wall has heat transport properties that were used to recreate the wall heat losses calculated by the corresponding model in a pressure trace analysis (PTA) [4, 18]. As a mass flow from the unburnt into the burnt zone is used in the Entrainment model to represent the combustion [4, 15], the same technique was chosen for the simulation model in this work. Blow-by losses were also considered by evaluating the mass flow rate through an orifice resulting from a pressure gradient [4]. The exhaust gas composition can be calculated from the surrogate component fractions and the AFR by assuming post-catalyst extraction. Thus, the initial conditions needed at simulation start are the mixture composition (surrogate component fractions, AFR and EGR rate) as well as the initial volume (piston position), pressure and temperature. The simulations yield if the mixture auto-ignites and when as well as the production and consumption of species causing changes in temperature and pressure. The model was validated by comparing simulated temperature profiles with PTA results in the compression stroke, where no heat release takes place. The curves showed very good agreement.

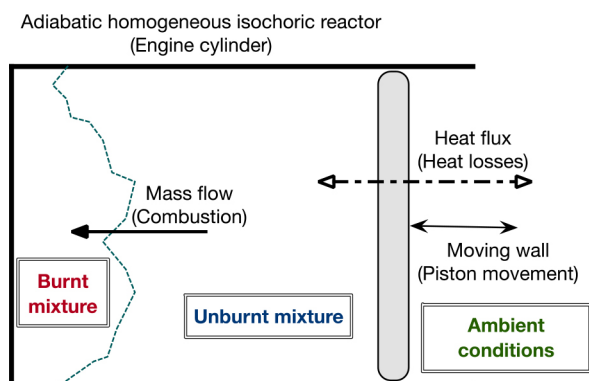


Figure 1. Model for reaction kinetic simulations at in-cylinder conditions.

Investigation Findings

By simulating thousands of working cycles at various boundary conditions, it was found out that the local auto-ignition in the unburnt mixture resulting in knock can occur in two stages. This phenomenon has already been observed in various studies in the context of gasoline Homogeneous Charge Compression Ignition (gHCCI) [10], but has not been extensively investigated in the context of engine knock. The temperature profiles shown in Figure 2 illustrate the two-stage ignition behavior. The phenomenon is related to the negative temperature coefficient (NTC) zone of the base fuel clearly visible in Figure 3, where the rate and extent of the hydrocarbon

oxidation reactions, which at first increase rapidly with temperature, begin to fall with further rise in the temperature, causing an increase in the ignition delay times in this temperature region [19].

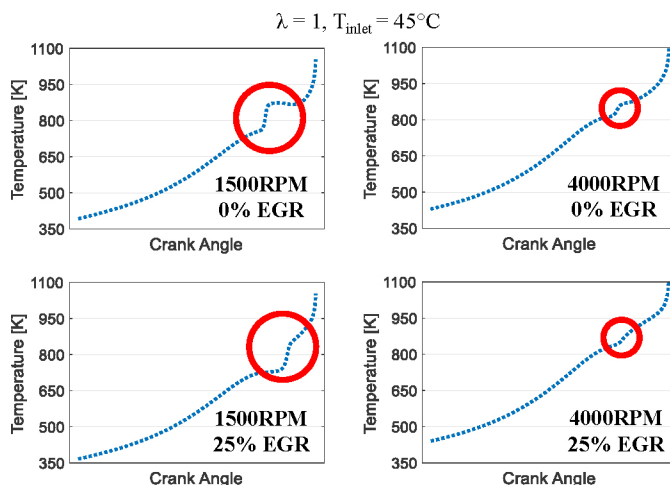


Figure 2. Simulated temperature profiles of different working cycles with auto-ignition in two stages depending on the boundary conditions.

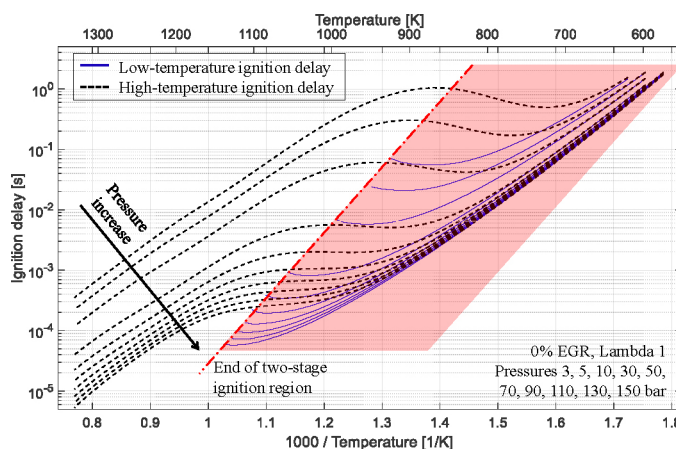


Figure 3. Two-stage ignition region and ignition delay times of the low- and high-temperature ignition regimes (base gasoline surrogate).

Obviously, the amount of heat released during the low-temperature (or the first stage of) ignition depends on the boundary conditions, e.g. engine speed and EGR rate as shown in Figure 2. Increasing engine speeds and high EGR rates cause the temperature rise resulting from the low-temperature ignition to decline. Generally, two-stage ignition behavior characterizes iso-octane and n-heptane [10]. As these two hydrocarbons, together with toluene and ethanol, compose the surrogate fuel, they also cause the observed low-temperature heat release. The resulting temperature increase accelerates the following chemical reactions. Thus, it influences the ignition delay of the mixture significantly [10].

The boundary condition region where two-stage ignition of the base fuel-air mixture investigated in this study occurs is illustrated in Figure 3. The existence of an ignition delay time of the low-temperature ignition primarily depends on temperature and pressure and defines the two-stage ignition region of a given surrogate composition. Hence, the influence of EGR and the fuel on the region's size can be neglected. Furthermore, Figure 3 clearly shows

that, at high temperatures, the two-stage ignition phenomenon does not occur at all. This observation is relevant for both knock and gHCCI operation with high internal EGR rates, as these lead to high temperatures of the unburnt mixture.

Knock Integral Auto-Ignition Prediction Performance

The ignition of the unburnt air-fuel mixture in two stages has a significant influence on the ignition delay. Hence, the question arises, if the commonly used knock integral can consider this effect and thus predict the auto-ignition location accurately in case the mixture ignites in two-stages. Figure 4 shows a comparison between the crank angles of knock onset (mixture auto-ignition) simulated with the detailed reaction kinetics mechanism at in-cylinder conditions and those predicted by a knock integral, equation (3), at various boundary conditions. The ignition delay times used as integral inputs were estimated by performing simulations with the detailed mechanism in an isochoric adiabatic reactor.

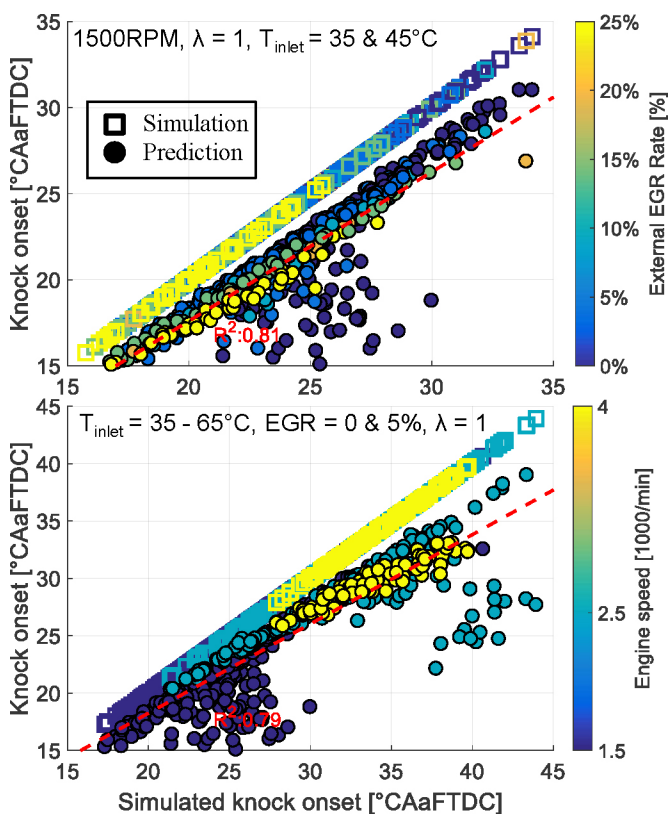


Figure 4. Crank angles of knock onset simulated with the detailed mechanism and predicted by a knock integral at various boundary conditions.

Obviously, the occurrence of two-stage ignition results in partially huge errors and hence poor performance of the knock onset prediction. The most significant prediction errors are in the regions where the low-temperature ignition leads to considerable heat release and thus temperature rise - low engine speeds and lack of EGR, see

Figure 2. Hence, the knock integral cannot account for the low-temperature ignition and its influence on the mixture's ignition delay. These results clearly show that the theoretical approach commonly used for modeling knock in 0D/1D SI engine simulations is not capable of reproducing the behavior of the detailed reaction kinetics mechanism at in-cylinder conditions. Hence, it is not a suitable replacement for the "detailed chemistry" and cannot be used for a reliable knock onset prediction in SI engines running on gasoline. The general knock modeling approach rather has to be changed or improved, in order to consider the occurrence of two-stage ignition.

TWO-STAGE IGNITION MODELING

An approach for modeling knock that accounts for a low-temperature ignition possibly taking place requires the development of suitable models for the three main parameters characterizing the two-stage ignition phenomenon. These are the ignition delay times of both ignition stages as well as the temperature increase resulting from the low-temperature ignition. First of all, the quantification of these three parameters is necessary.

Definitions

The values of the parameters characterizing the two-stage ignition phenomenon were obtained in Cantera/Matlab simulations of an isochoric adiabatic homogeneous reactor with the detailed mechanism already brought up in the previous section. An algorithm based on the production of OH radicals followed by their consumption and consequentially temperature increase before the mixture's auto-ignition detected the occurrence of two-stage ignition. In this work, the delays of the two ignition stages and the temperature increase resulting from the low-temperature ignition were defined as follows (Figure 5):

- The location of the low-temperature ignition and hence the low-temperature ignition delay τ_{low} is defined as the point $\max(T_{grad})$, where the temperature gradient reaches its maximum before the auto-ignition of the mixture.
- The high-temperature or the auto-ignition delay τ_{high} is detected based on a threshold for the temperature gradient. This method has already been suggested in other studies [13]. The value of the temperature gradient threshold was set to 25 K/microsecond.
- The temperature increase T_{incr} resulting from the low-temperature ignition is defined as temperature at simulation start subtracted from the temperature at the point $\min(T_{grad})$, where the temperature gradient reaches its minimum between the two ignition stages. This definition has already been suggested in previous studies [12].

A variable simulation step was implemented to save computational time. The boundary conditions were varied according to in-cylinder values typical for SI engines today with the main goal being to cover

a sensible value range as wide as possible. Therefore, pressures of up to 150 bar, high unburnt mixture temperatures of up to 1300 K, air-fuel equivalence ratios λ in the interval 0.7 - 1.5 with exhaust gas mass fractions of up to 30% and ethanol contents between 0% and 20% were simulated. Obviously, the exhaust gas composition has to be changed in accordance with the AFR. Moreover, the fractions of the three base surrogate components (iso-octane, n-heptane and toluene) were varied too, as only one, specific surrogate composition is representative for a given gasoline fuel and matches up to its characteristics. This representative surrogate composition can be calculated from fuel parameters such as the Research and Motor Octane Numbers (RON and MON), density, or lower heating value with the corresponding blending rules [5, 6, 7].

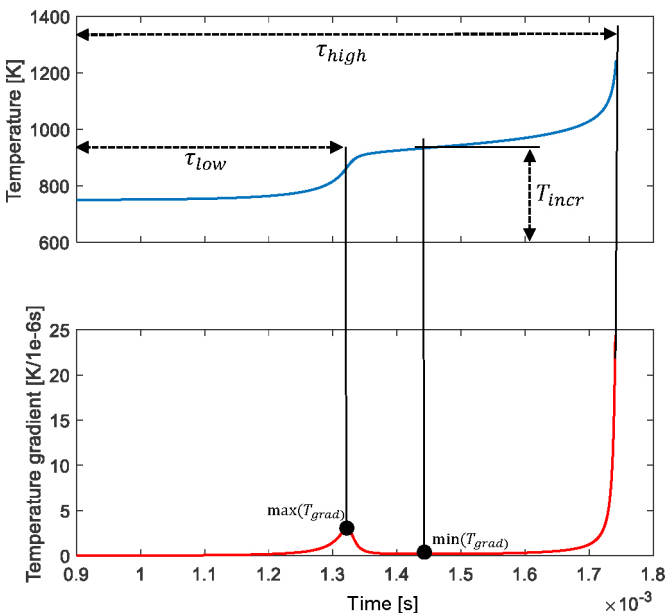


Figure 5. Definition of low- and high-temperature ignition as well as the temperature increase resulting from the first ignition stage in an adiabatic isochoric reactor at 750K, 70bar and $\lambda = 1$, no exhaust gas mass present.

The simulation results show that generally, the ignition delay times of both ignition changes decrease with pressure and increase with the exhaust gas mass fraction and AFR, see Figures 6 and 7. Moreover, rising λ as well as the presence of exhaust gas lead to a lower temperature increase resulting from the low-temperature ignition. In contrast, higher pressures cause the temperature increase to rise, Figure 8. Clearly, the NTC zone has to be modeled as precisely as possible because of its significant influence on the ignition delay times. The simulation data were used to develop new models for the calculation of the three main parameters characterizing the two-stage ignition phenomenon, with the two main goals being the achievement of high accuracy of the calculated values and short computational times. The developed models can afterwards be installed in a new knock modeling approach that accounts for the possible occurrence of two-stage ignition and its influence on the mixture's ignition delay.

All estimated model parameters should only be recalibrated if values of the parameters characterizing the two-stage ignition phenomenon obtained with a reaction kinetics mechanism different than the one used in this work have to be considered.

High-Temperature Ignition Delay

In [8], a distinction between low-, medium- and high-temperature regimes of ignition is proposed, resulting in a 3-domain approach for the calculation of the ignition delay times of an air-fuel mixture. Hence, the high-temperature ignition delay can be expressed as shown in equation (4). This correlation is particularly suitable for fuels with clearly visible negative temperature coefficient behavior.

$$\frac{1}{\tau_{high}} = \frac{1}{\tau_{1,high}} + \frac{1}{\tau_{2,high}} + \frac{1}{\tau_{3,high}} \quad (4)$$

$\tau_{1,high}$, $\tau_{2,high}$ and $\tau_{3,high}$ represent ignition delays of the mixture in the low-, medium- and high-temperature regimes of ignition respectively. Each of these three timescales can be evaluated using a single Arrhenius-type correlation, similar to equation (2). Generally, this equation is expanded by adding parameters in front of the exponential function to account for the influence of various changes in the boundary conditions on the mixture's ignition delay. However, it is much more convenient to put these together in just two parameters $A_{i,high}$ and $B_{i,high}$ with i denoting the temperature regime, leading to a simpler equation form and a more flexible triple-Arrhenius approach, equation (5).

$$\tau_{i,high} = A_{i,high} \cdot e^{\left(\frac{B_{i,high}}{T}\right)}, A_{i,high}, B_{i,high} = f(p, \lambda, EGR, fuel) \quad (5)$$

This enhanced approach has already been proposed by the authors of this work in [14]. It has the major advantage over the commonly used correlation in equation (2) and its variations that it can be fitted to much more complexly shaped ignition delay curves, as in the case of this study, Figure 6. Furthermore, as the numerator in the exponential function in equations (2) and (5) respectively is proportional to the activation energy needed for the aggregate reaction to take place and the auto-ignition to occur, changes in the boundary conditions are reflected in different values of the activation energy in equation (5). In contrast, the activation energy in equation (2) remains constant for each temperature regime, leading to an error that has to be corrected by the coefficients in front of the exponential function. Disadvantageous is that, partially because of its flexibility, the approach proposed here is more difficult to fit to simulation data.

However, the estimation of the empirical parameters in equation (5) was fully automated in Matlab. Furthermore, an automatic optimization of the estimated values was implemented by using the algorithm described in [9] to minimize the normalized root mean

square deviation of the empirically calculated ignition delay times. The implemented normalization accounts for the different magnitudes of the values of the ignition delay times. The enhanced 3-domain approach, together with the implemented parameter optimization, result in a new high-temperature ignition delay model that yields results with very high accuracy, as shown in Figure 6 for the chosen base E10 gasoline fuel. All model equations and parameters are listed in the [Appendix](#). Additionally, a validation of the modeled influence of the surrogate composition on the high-temperature ignition delay times is shown in [Figure A1](#).

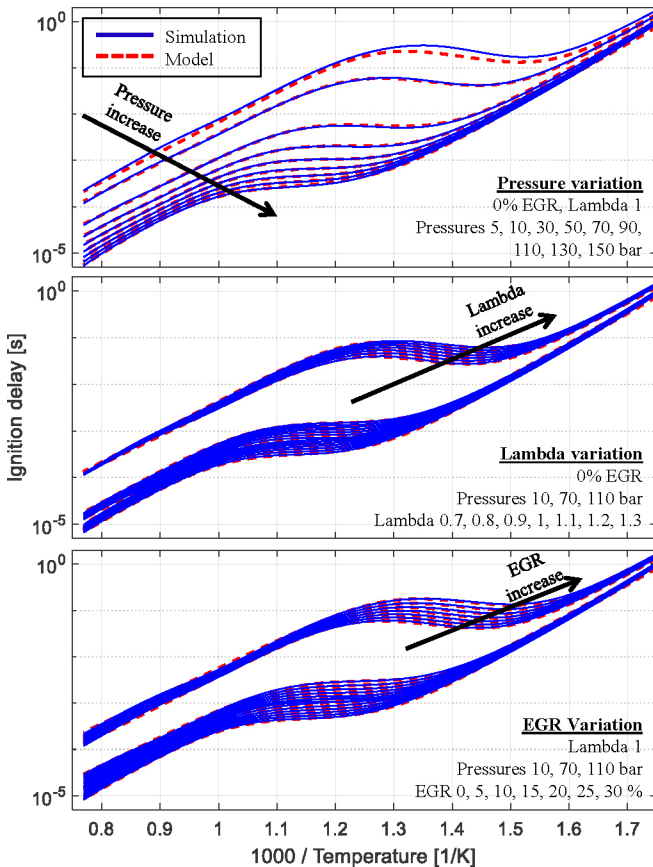


Figure 6. Simulated and modeled high-temperature ignition delay times at various boundary conditions (base gasoline surrogate).

Low-Temperature Ignition Delay

For the low-temperature ignition delay τ_{low} , it is convenient to choose a modeling approach similar to the one for the auto-ignition delay times. Obviously, the low-temperature ignition delay curves shown in [Figures 3](#) and [7](#) are characterized by just two temperature regimes of ignition. Hence, the modeling approach has to account for the low and medium regimes only, [equation \(6\)](#). As is the case in [equation \(5\)](#), the Arrhenius-type correlations for the two low-temperature ignition temperature regimes include two parameters $A_{i,low}$ and $B_{i,low}$ that change with the boundary conditions, [equation \(7\)](#). Thus, alternations in the boundary conditions are reflected in an activation energy change.

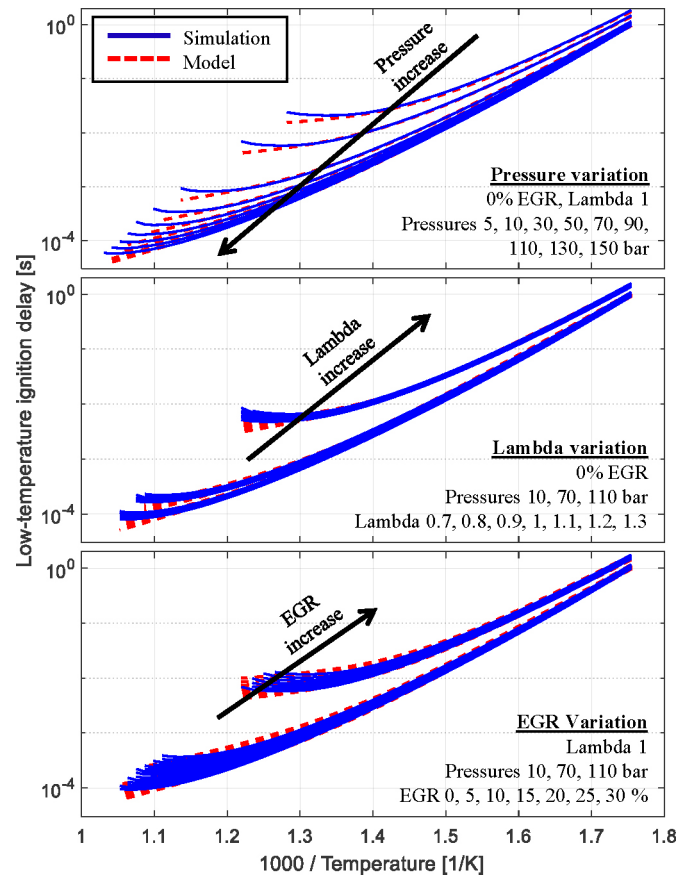


Figure 7. Simulated and modeled low-temperature ignition delay times at various boundary conditions (base gasoline surrogate).

$$\frac{1}{\tau_{low}} = \frac{1}{\tau_{1,low} + \tau_{2,low}} \quad (6)$$

$$\tau_{i,low} = A_{i,low} \cdot e^{\left(\frac{B_{i,low}}{T}\right)}, A_{i,low}, B_{i,low} = f(p, \lambda, EGR, fuel) \quad (7)$$

The parameter estimation and optimization techniques used in the low-temperature ignition delay model do not differ from those already discussed in the high-temperature ignition delay section. Thus, high accuracy of the calculation results could be achieved, [Figure 7](#). All model equations and parameters as well as a validation of the modeled surrogate composition influence on the low-temperature ignition delay times can be found in the [Appendix](#), [Figure A2](#).

Temperature Increase Resulting from Low-Temperature Ignition

The occurrence of low-temperature ignition results in heat release, leading to a temperature increase. Hence, there is one temperature increase value corresponding to every existing low-temperature ignition delay. As the occurrence of two-stage ignition and thus the presence of a low-temperature ignition delay are primarily influenced by temperature and pressure, these two parameters are also decisive for the existence of a value for the temperature increase.