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Correlations for the Laminar Flame Speed, Adiabatic Flame Temperature and Ignition Delay Time for methane, ethanol and n-decane

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This paper provides a detailed database for curve fitted polynomials to deliver information about the laminar flame speed, adiabatic flame temperature and ignition delay time depending on the equivalence ratio, temperature and pressure. The fuels under investigation are methane, ethanol and n-decane. A new aspect of this paper is the envisaged broad range of validity of the correlations, covering the range of 0.6 - 1.5 for the equivalence ratio, 293.15 K - 593.15 K for the temperature, regarding the laminar flame speed and the adiabatic flame temperature and 1400 K - 1800 K, regarding the ignition delay time and 0.5 bar - 6 bar for the pressure range. As basis of the mathematical expressions, curves with the highest order of four have been chosen to best describe the behavior of the quantities under examination. Evaluation of well established experimental data sets for each respective fuel generates a first rudimentary groundwork for the derivation of the polynomial. The experimental results are further enhanced by obtaining a large amount of additional points through finite rate chemistry simulations with detailed reaction mechanism. By means of a least squares fit, the coefficients for the algebraic expression are inferred. An error analysis is contained subsequent to the calculation, helping the reader to assess the reliability and quality of the fitted curves.

Nomenclature

Variables

A	Cross Section [m^2]				
c_p	Heat Capacity at Constant Pressure [J/kgK]				
C	Polynomial Coefficients [-]	D	Deviation [Unit]	h	Specific Enthalpy [J/kg]
I	Identity Matrix [-]	J	Jacobian Matrix [Unit/Unit]		
k	Number of Coefficients [$-$]	λ	Heat Transfer Coefficient [W/mK]		
m	Number of Reactions [$-$]	$\dot{M}$	Mass Flow Rate [kg/s]	n	Number of Species [$-$]
N	Number of Nodal Points	ω	Reaction Rate [Unit/s]	ϕ	Equivalence Ratio [-]
p	Pressure [Pa]	R	Ideal Gas Constant [J/molK]		
t	Time [s]	T	Temperature [K]	V	Diffusion Velocity [m/s]
W	Molecular Weight [kg/mol]	y	Function Variable [Unit]	Y	Mass Fraction [$-$]
Z	Result Matrix [Unit]				

Indices

a	Approximated Value	e	Exact Value	i	Index Variable [-]
j	Index Variable [-]				

Systematics

$\vec{}$	Vector	$\underline{\underline{}}$	Matrix	$'$	Transpose

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I. Introduction

The recent development in numerical activities has shown that there is still a huge need for simplified chemistry models. When looking at the rapid growth in LES applications, the required computational power to calculate only the fundamental quantities of the flow field is immense, impeding the use of a complex chemical scheme. Since several simplified chemistry models, as for example the Turbulent Flame Speed Closure model and the G-Equation model, rely on the laminar flame speed as one of the inherent scaling factors, a large implementation aid is, to have a sound mathematical expression available. Although some material is already available on this topic, for example by Mueller et al.[1] for methane and Liao et al.[2] for ethanol, none attempts to span the whole equivalence range or do not include the fuels described in this survey. In this paper three main representatives are chosen, with methane being one of the important fuels in pure gaseous simulations and with ethanol and n-decane offering an option of modeling combustion under multiphase flow conditions. Therefore, this paper provides polynomial fitted curves for the laminar flame speed, the ignition delay time and the adiabatic flame temperature, all representing crucial flame characteristic properties. Analysis of data for the all three quantities has resulted in choosing polynomials with a maximum order of four to be appropriate for reproducing the right values over a broad range. Hence, the general expression extracted from a set of nodal points is conducted in the functional form of $y = \mathrm{f}(\phi, T, p)$. The approach taken to derive the final correlation coefficients is the following. Reaction schemes derived by kinetic analysis and by adaptation with experimental data are employed as the basis for the calculation of a multitude of nodes. These serve as input into a least squares fitting routine which delivers the coefficients for the algebraic expression.

II. Model

In this section the necessary steps to derive the final curve coefficients are described. The first task is the analysis of a variety of possible reaction schemes for each respective fuel. By comparison of the performance of computed results with the measured data, the choice of an appropriate chemical mechanism for the derivation of additional nodes is achieved. With the respective mechanism a series of simulations is carried out to gain a thorough database for the later establishment of the polynomial coefficients. The purpose of an extended data base for the correlation lies in the enhanced probability of matching the right course and in the incorporation of data intervals which might for some reason not be measured. This could happen near the flammability limits where sometimes no stable flame could be accomplished experimentally. Fig. (1) elucidates the problematic faced in deriving an appropriate polynomial in case too few data points are available.

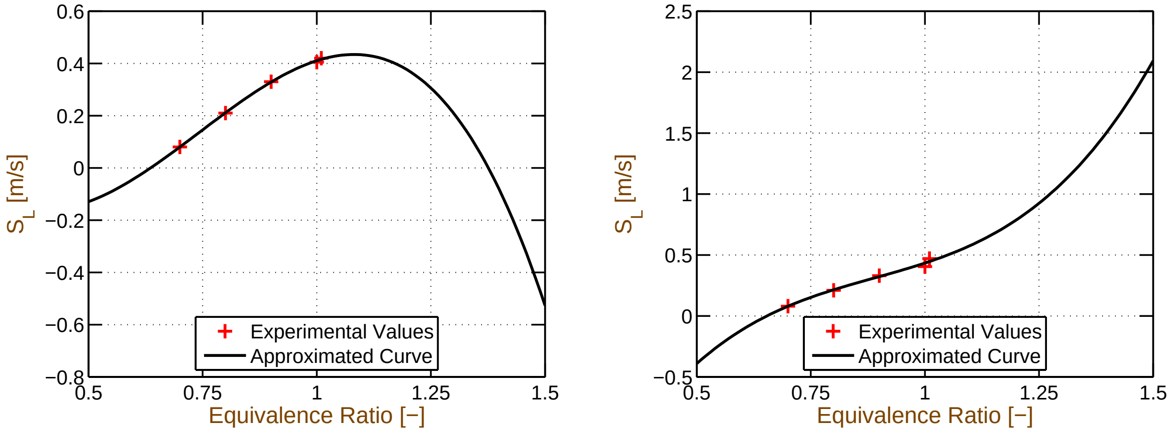

Figure 1. Exemplary demonstration of an approximation with only 5 data points. Results show the large influence of the location of the nodes. Slight differences lead to a dramatic change in the course of the least squares curve.

II.A. Generation of Data Points for the Ignition Delay Time

The solution process for the ignition delay time is based on the assumption of a perfectly stirred, adiabatic, isobaric reactor. The calculation are carried out with a numerical tool called int0D which is originates from the finite rate chemistry model of the in-house code THETA. For the evolution of the chemical reactions a finite rate chemistry solver is employed. Some of the fundamental equations, underlying the approach shall be described shortly. For any chemical systems, a problem involving n unknowns for the n species and the temperature, whereby the last species can be calculated by $Y_n = 1 - \sum_{i=1}^{n-1} Y_i$, and m reactions is faced. Denoting the vector of unknowns:

$$\vec{\Psi} = \begin{Bmatrix} Y \\ T \end{Bmatrix}, \tag{1}$$

the evolution of the composition is given by the ODE: $\partial\vec{\Psi}/\partial t = \vec{\omega}$ with the initial conditions specified as $h = h(t_0) = \text{const.}$ and $p = p(t_0) = \text{const.}$. The system of ODEs is solved numerically. In order to increase the stability, an implicit approach was chosen which also helps to avoid problems with very small time step sizes necessary in an explicit scheme. Thus, this yields for the ith source term:

$$\omega_i(\vec{\Psi}^{t+\Delta t}) = \omega_i\left(\vec{\Psi}^t\right) + \left|\frac{\partial\omega_i}{\partial\vec{\Psi}}\right|^t \Delta\vec{\Psi} + \mathcal{O}(||\Delta\vec{\Psi}||^2) \tag{2}$$

where $\frac{\partial\omega_i}{\partial\Psi}$ is the i-th line of the Jacobian matrix, calculated at time t. A semi implicit Euler method is employed, as method to derive the solution at the new time step, giving:

$$\begin{aligned} \left(\frac{1}{2}\underline{\underline{J}}^t - \frac{\underline{\underline{I}}}{\Delta t}\right)\Delta\vec{\Psi} &= -\vec{\omega}^t \\ \Psi_i^{t+\Delta t} &= \Psi_i^t + \Delta\Psi_i \end{aligned} \tag{3}$$

More details on this topic can be found in the work of Di Domenico[3] and Gerlinger.[4]
Hence, with accurately defined initial conditions, the chemical reaction is started at the time $t = 0$ s with the purpose of extracting the position of the largest incline in the temperature profile. The slow increase shortly before the intense exothermal reaction starts does not influence the procedure neither does the slow balancing-out of the last reactions. By determining the occurrence of the sharpest increase in the profile, an exact value of the ignition delay time for a corresponding data set of T, ϕ and p can be derived.

II.B. Generation of Data Points for the Adiabatic Flame Temperature

For the purpose of generating additional nodes for the adiabatic flame temperature, the governing equations as described in the previous subsection are solved until equilibrium. Hence, the source term ω_i for all i unknowns must converge to zero. The temperature in the converged solution constitutes the adiabatic flame temperature for a given set of initial conditions.

II.C. Generation of Data Points for the Laminar Flame Speed

The extraction of additional nodes for the laminar flame speed represents a more sophisticated challenge in fundamental kinetic simulations. The employed numerical tool is a Cantera based source code. Unlike to the previous task in which a perfectly stirred reactor with appropriate accuracy would lead to readily interpretable results, this is more advanced when inferring on the flame speed. The approach employed in this paper is based on a one-dimensional laminar premixed flame configuration. Several authors, for example Grcar,[5] Smooke[6] and Peters[7] have established valuable knowledge on this field. The underlying equations have the following form:

$$\dot{M} = \rho u A = \text{constant} \tag{4}$$

$$\dot{M}\frac{\partial T}{\partial x} - \frac{1}{c_p}\frac{\partial}{\partial x}\left(\lambda A\frac{\partial T}{\partial x}\right) + \frac{A}{c_p}\sum_{i=1}^{n}\rho Y_i V_i c_{p_i}\frac{\partial T}{\partial x} + \frac{A}{c_p}\sum_{i=1}^{n}\dot{\omega}_i h_i W_k = 0 \tag{5}$$

$$\dot{M}\frac{\partial Y_i}{\partial x} + \frac{\partial}{\partial x}\left(\rho A Y_i V_i\right) - A\dot{\omega}_i W_i = 0 \ (i = 1, ..., n) \tag{6}$$

The difficult task is thus, to find the eigenvalue of $\dot{M}$ which solves the above stated system of equations. For this reason, boundary conditions need to be prescribed and a discretization must be accomplished. Details on this procedure can be found in the work of Smooke.[6] As the whole problem is very sensitive to the initial guess, a multi staged approach, corresponding to the one proposed by Smooke[6] is utilised. The different steps until a converged solution is obtained, can be categorized as:

- Derivation of an initial frozen solution with a fixed temperature profile and a fixed mass flow. Grid points are inserted at intervals with large fluctuation between iterations.
- Determination of an initial solution including chemical reactions. Receipt of a first good guess for further "hot" iterations.
- Continue to refine grid in intervals with large deviations until a stable converged solution is obtained.

Finally, the value of the laminar flame speed can be extracted to be used for the generation of an adequate number of nodal points, which are required for the least squares fitting.

II.D. Least Squares Fit of Data

The methods described in this section mostly belong to the category "basic fundamental mathematical tools". Nevertheless, for completeness and for a thorough understanding of the origin of the polynomial coefficients, the approach shall be shortly elucidated here. With the routines discussed in the earlier subsections which were all devoted to the generation of additional nodal points, a set of equation can be compiled for the least squares fit. Some comprehensive literature on this topic can be found in the work of Bjoerck,[8] Rao[9] and Kariya.[10] For each nodal point i, the deviation between correlation and the correct value can be written as:

$$D_i = y_{e_i} - y_{a_i}(T_i, p_i, \phi_i) \tag{7}$$

As y_{a_i} represents the approximated node, a sensible expression needs to be proposed for the calculation. The authors have decided to employ functions of the form: $y_{\mathrm{a}_i} = \sum_{j=1}^{k} C_j^\star \cdot f_j(T_i, p_i, \phi_i)$ to be well suited for this kind of task.

Hence, the objective is to determine the unknown coefficients for the entire range of p, T and ϕ. For conciseness and in order to simplify the mathematical operations, matrix and vector notation is introduced. The coefficient and state vector can be expressed as:

$$\vec{C}^\star = \left\{\begin{matrix} C_1^\star \\ C_2^\star \\ \vdots \\ \vdots \\ C_n^\star \end{matrix}\right\} \qquad \vec{Z}_i = \left\{\begin{matrix} f_1(T_i, p_i, \phi_i) \\ f_2(T_i, p_i, \phi_i) \\ \vdots \\ \vdots \\ f_n(T_i, p_i, \phi_i) \end{matrix}\right\} \qquad \begin{matrix}\text{with any} \\ \text{approximated node} \\ \text{assembled as:}\end{matrix} \qquad y_{\mathrm{a}_i} = \vec{Z}_i'\vec{C}^\star \tag{8}$$

For the entity of all deviations from the fixed nodal values we can write:

$$D_i = y_{e_i} - \vec{Z}_i'\vec{C}^\star \tag{9}$$

which can be conveyed to a single expression:

$$\vec{D} = \vec{y}_e - \underline{\underline{Z}}\vec{C}^\star \tag{10}$$

By taking the square of both sides, the initial formulation of the least squares problem is accomplished. As the aim is to derive the minimum of the least squares function regarding the coefficient vector, the D^2 expression is to be derived once with respect to the coefficient vector. This yields:

$$\frac{\partial}{\partial \vec{C^\star}} \vec{D}' \vec{D} = 0 = -\underline{\underline{Z}} \vec{y}_e + \underline{\underline{Z Z}} \vec{C^\star} \tag{11}$$

with the final expression for $\vec{C^\star}$:

$$\vec{C^\star} = \underline{\underline{Z}}^{-1} \vec{y}_e \tag{12}$$

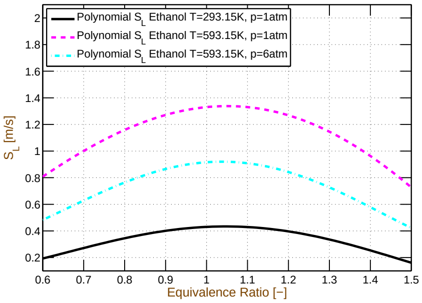

Figure 2. Plot of S_L of ethanol for different pressures and temperatures. Strong variations in the course prevail.

For obtaining the inverse of the state matrix the Singular Value Decomposition scheme is applied. As courses of the laminar flame speed differ strongly within the envisaged pressure and temperature range, s. Fig. (2), a set of 45 coefficients is necessary to preserve a satisfying accuracy in the chosen range. Multiple approaches have been evaluated, leading to the final expression which involves terms of the order of four. In order to simplify the notation several coefficients are combined to yield an auxiliary coefficient, e.g. according to Eq. 13 for the laminar flame speed. This simplifies the derived function to Eq. 14 in case of the laminar flame speed. The same simplification process is adapted for the ignition delay time and the adiabatic flame temperature.

$$\begin{aligned} C_i \quad &= C^\star_{i,1} \quad && +C^\star_{2_i} T + C^\star_{i,3} T^2 + C^\star_{i,4} T^3 \\ & && +C^\star_{i,5} T^4 + C^\star_{i,6} p + C^\star_{i,7} p \cdot T \\ & && +C^\star_{i,8} p \cdot T^2 + C^\star_{i,9} p^2 \cdot T^2 \text{ for } i = 1...5 \end{aligned} \tag{13}$$

$$S_\mathrm{L} = C_1 + C_2 \phi + C_3 \phi^2 + C_4 \phi^3 + C_5 \phi^4 \tag{14}$$

Note, that for conciseness, the vector $\vec{C^\star}$ is rearranged to a matrix which is more convenient for the annotation. E.g., $C^\star_{2,2}$ denotes the eleventh element of the coefficient vector, whereas $f_{2,2} = \phi T$ according to Eq. 8, Eq. 13 and Eq. 14.

III. Results

This section is dedicated to the presentation of the outcome of the derived polynomials by the least squares fits. For each of the fuels a separate subsection is provided to simplify the look up of curve coefficients. For each quantity, namely, the laminar flame speed, the ignition delay time and the adiabatic flame temperature a second subdivision is performed. At the end of each part a short error analysis with respect to the deviation of the polynomial approximation to the nodal points for a particular constant temperature, pressure and equivalence ratio is accomplished to support an accurate judgment of the agreement. Generally, the coefficients are provided to the fourth/fifth digit which is a round-off of the exact value which is accounted for in the error analysis.

The error which is presented for all investigated fuels and quantities is derived in the following manner. For a particular value of one quantity the other two parameters are varied, according to the number of available nodal points to yield to total error. Consequently, the formulae for the error calculation read:

$$\begin{aligned} Dy_{p_K} &= \sum_{i=1}^{N_T} \sum_{j=1}^{N_\phi} |y_\mathrm{e}(T_i, p_K, \phi_j) - y_\mathrm{a}(T_i, p_K, \phi_j)| / (N_T + N_\phi) \\ Dy_{T_K} &= \sum_{i=1}^{N_p} \sum_{j=1}^{N_\phi} |y_\mathrm{e}(T_K, p_i, \phi_j) - y_\mathrm{a}(T_K, p_i, \phi_j)| / (N_p + N_\phi) \\ Dy_{\phi_K} &= \sum_{i=1}^{N_p} \sum_{j=1}^{N_T} |y_\mathrm{e}(T_j, p_i, \phi_K) - y_\mathrm{a}(T_j, p_i, \phi_K)| / (N_p + N_T) \end{aligned} \tag{15}$$

In Eq. 15, y_{p_K}, y_{T_K} and y_{ϕ_K} represent the values computed for a particular value of either p, T or ϕ. The error is, thus, accumulated over all available nodal points for this particular value and divided by the amount (N_T, N_ϕ, N_p) of all considered nodal points which gives the averaged error.

The range covered for each respective quantity are, for the temperature: 293.15 K $< T <$ 593.15 K, for the equivalence ratio: $0.6 < \phi < 1.5$ and for the pressure: 0.5 bar $< p <$ 6.0 bar.

III.A. methane

In the case of a methane flame the GRI3.0[11] mechanism is employed for the calculation of additional nodal points.

III.A.1. Laminar Flame Speed

Figure (3) shows the behavior of the laminar flame speed for a number of varied conditions. For different values of p and T, a good agreement is achieved for the entire equivalence ratio range. As the polynomial is established using nodal points in the lean and rich regime, the approximation is suitable for complex configurations covering a broad range of equivalence ratios. The error introduced by the polynomial with respect to the derived nodal points is listed in Table 1. The final coefficients are provided in Table 2.

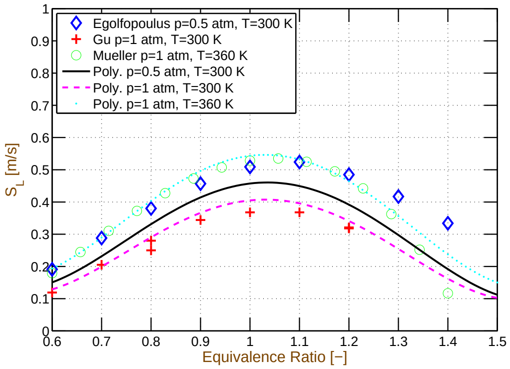

Figure 3. Comparison of values derived with the polynomial with literature data. The first set of experimental values is taken from Egolfpopoulus et al.[12] The second data set originates from the work of Gu et al.[13] The last set compares the polynomial proposed by Mueller et al.,[1] valid under lean conditions, with the present polynomial.

T[K]	D[m/s]	p[bar]	D[m/s]	ϕ[-]	D[m/s]
293.15	1.03e-2	0.5	4.25e-2	0.6	1.55e-2
343.15	1.23e-2	1.0	1.86e-2	0.7	1.88e-2
393.15	1.47e-2	1.5	2.93e-2	0.8	1.84e-2
443.15	1.74e-2	2.0	2.36e-2	0.9	2.01e-2
493.15	2.03e-2	2.5	1.33e-2	1.0	1.90e-2
543.15	2.37e-2	3.0	8.75e-3	1.1	1.86e-2
593.15	2.72e-2	3.5	1.10e-2	1.2	1.75e-2
		4.0	1.48e-2	1.3	1.97e-2
		4.5	1.50e-2	1.4	2.05e-2
		5.0	1.00e-2	1.5	1.18e-2
		5.5	7.53e-3		
		6.0	2.14e-2		

Table 1. The error at a constant temperature, pressure and mixture fraction is calculated according to Eq. 15.

III.A.2. Ignition Delay Time

A comparison between experimental data and calculated ignition delay times is presented in Fig. (4) for two different pressures and equivalence ratios with varying temperature. The first curve demonstrates the good quality of the polynomial with respect to capturing the ignition delay time within the investigated temperature range for an equivalence ratio of 0.5 for a methane/Air mixture at 3.3 bar. The second comparison contains data from Seery et al.[14] for a diluted methane/Air/Argon mixture which underlines the accuracy of the nodal points. Note, that since diluted mixtures are not contained in the derivation of the polynomial no direct comparison with the results from Seery et al.[14] can be accomplished. The error which occurs in approximated the nodal points is given in Table 3. The derived coefficients are provided in Table 4.

III.A.3. Adiabatic Flame Temperature

The adiabatic flame temperature has been approximated in the entire condition range. The agreement as depicted in Fig. (5) is of very satisfying quality. The experimental data stemming form Kishore Ratna[16] et al. is well matched and, moreover, the approximation by Mueller et al.[1] is reproduced well, too. Note, that the correlation proposed by Mueller et al.[1] is only valid in the lean regime, clarifying why deviations

Coefficients for the Laminar Flame Speed

General Form: $S_{\mathrm{L}} = C_1 + C_2\phi + C_3\phi^2 + C_4\phi^3 + C_5\phi^4$

Correlation for C_i

Formulation: $C_i = C^\star_{i,1} + C^\star_{i,2}T + C^\star_{i,3}T^2 + C^\star_{i,4}T^3 + C^\star_{i,5}T^4 + C^\star_{i,6}p + C^\star_{i,7}p \cdot T + C^\star_{i,8}p \cdot T^2 + C^\star_{i,9}p^2 \cdot T^2$

Note, T/300 [K], p/1e5 [Pa].

$C^\star_{1,1}$:	1.80952e+01	$C^\star_{2,1}$:	-7.94577e+01	$C^\star_{3,1}$:	1.27177e+02	$C^\star_{4,1}$:	-8.76212e+01	$C^\star_{5,1}$:	2.18831e+01
$C^\star_{1,2}$:	-4.71247e+01	$C^\star_{2,2}$:	2.06418e+02	$C^\star_{3,2}$:	-3.29619e+02	$C^\star_{4,2}$:	2.27222e+02	$C^\star_{5,2}$:	-5.68799e+01
$C^\star_{1,3}$:	5.45663e+01	$C^\star_{2,3}$:	-2.41694e+02	$C^\star_{3,3}$:	3.89192e+02	$C^\star_{4,3}$:	-2.68602e+02	$C^\star_{5,3}$:	6.69844e+01
$C^\star_{1,4}$:	-2.65938e+01	$C^\star_{2,4}$:	1.17837e+02	$C^\star_{3,4}$:	-1.89151e+02	$C^\star_{4,4}$:	1.30348e+02	$C^\star_{5,4}$:	-3.25052e+01
$C^\star_{1,5}$:	4.46007e+00	$C^\star_{2,5}$:	-1.97134e+01	$C^\star_{3,5}$:	3.16725e+01	$C^\star_{4,5}$:	-2.18638e+01	$C^\star_{5,5}$:	5.46381e+00
$C^\star_{1,6}$:	-2.82275e−01	$C^\star_{2,6}$:	1.07488e+00	$C^\star_{3,6}$:	-1.70663e+00	$C^\star_{4,6}$:	1.27096e+00	$C^\star_{5,6}$:	-3.57336e−01
$C^\star_{1,7}$:	-4.80988e−01	$C^\star_{2,7}$:	2.53649e+00	$C^\star_{3,7}$:	-4.12943e+00	$C^\star_{4,7}$:	2.56811e+00	$C^\star_{5,7}$:	-5.22612e−01
$C^\star_{1,8}$:	1.02333e+00	$C^\star_{2,8}$:	-4.64311e+00	$C^\star_{3,8}$:	7.04341e+00	$C^\star_{4,8}$:	-4.58136e+00	$C^\star_{5,8}$:	1.08511e+00
$C^\star_{1,9}$:	-8.77924e−02	$C^\star_{2,9}$:	3.84077e−01	$C^\star_{3,9}$:	-5.72559e−01	$C^\star_{4,9}$:	3.76381e−01	$C^\star_{5,9}$:	-9.20466e−02

Table 2. Coefficients of the polynomial for the laminar flame speed of methane

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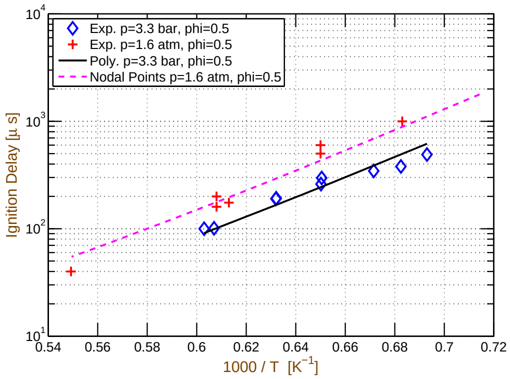

Figure 4. The first comparison is based on methane-air ignition delay times measured by Sechenov et al.[15] with the polynomial. The second comparison which shows measurement data from Seery et al.[14] and the corresponding nodal points underlines the good performance of the GRI3.0 mechanism.

T[K]	D[s]	p[bar]	D[s]	ϕ[-]	D[s]
293.15	1.22e-4	0.5	4.49e-5	0.6	2.09e-5
343.15	6.54e-5	1.0	5.42e-5	0.7	2.30e-5
393.15	3.51e-5	1.5	5.23e-5	0.8	2.49e-5
443.15	1.85e-5	2.0	3.85e-5	0.9	2.71e-5
493.15	9.79e-6	2.5	2.39e-5	1.0	2.88e-5
543.15	5.17e-6	3.0	1.13e-5	1.1	3.08e-5
593.15	3.03e-6	3.5	2.28e-6	1.2	3.20e-5
		4.0	9.80e-6	1.3	3.39e-5
		4.5	1.84e-5	1.4	3.55e-5
		5.0	2.59e-5	1.5	3.68e-5
		5.5	3.24e-5		
		6.0	3.84e-5		

Table 3. The error at a constant temperature, pressure and equivalence ratio is calculated according to Eq. 15.

Coefficients for the Ignition Delay Time

General Form: $t_{\mathrm{i}} = C_1 + C_2\phi$

Correlation for C_i

Formulation: $C_i = C^\star_{i,1} + C^\star_{i,2} \cdot 1/T + C^\star_{i,3} \cdot 1/T^2 + C^\star_{i,4} \cdot 1/T^3 + C^\star_{i,5} \cdot 1/T^4 + C^\star_{i,6} \cdot 1/p$
$+ C^\star_{i,7} \cdot 1/(p \cdot T) + C^\star_{i,8} \cdot 1/(p \cdot T^2) + C^\star_{i,9} \cdot 1/(p \cdot T^3) + C^\star_{i,10} \cdot 1/(p \cdot T^4)$

Note, T/1000 [K], p/1e5 [Pa].

Note, coefficients are written in row formation.

$C^\star_{1,1}$:	2.39005e−02	$C^\star_{1,2}$:	-1.74903e−01	$C^\star_{1,3}$:	4.79014e−01	$C^\star_{1,4}$:	-5.82448e−01	$C^\star_{1,5}$:	2.65583e−01
$C^\star_{1,6}$:	3.39938e−01	$C^\star_{1,7}$:	-2.26768e+00	$C^\star_{1,8}$:	5.68183e+00	$C^\star_{1,9}$:	-6.34326e+00	$C^\star_{1,10}$:	2.66631e+00
$C^\star_{2,1}$:	1.75173e−02	$C^\star_{2,2}$:	-1.22666e−01	$C^\star_{2,3}$:	3.26076e−01	$C^\star_{2,4}$:	-3.90313e−01	$C^\star_{2,5}$:	1.77613e−01
$C^\star_{2,6}$:	4.27790e−01	$C^\star_{2,7}$:	-2.90319e+00	$C^\star_{2,8}$:	7.39537e+00	$C^\star_{2,9}$:	-8.38286e+00	$C^\star_{2,10}$:	3.56882e+00

Table 4. Coefficients of the polynomial for the ignition delay time of methane.

are likely to occur towards richer conditions. The encountered error within the whole investigated range is fairly low, as shown in Table 5. The final coefficients of the polynomial are provided in Table 6.

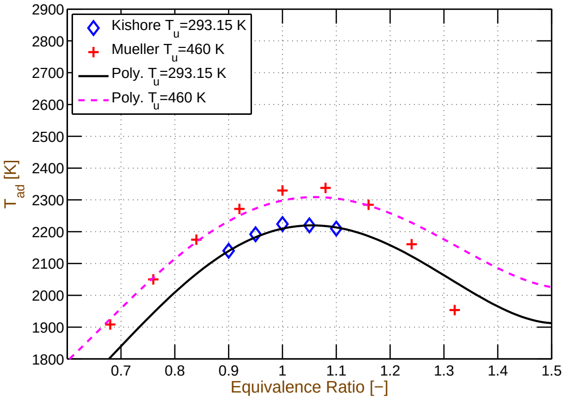

Figure 5. Comparison of the polynomial approximation with measurements from Kishore Ratna et al.[16] The second comparison is carried out with the approximation provided by Mueller et al.[1]

T[K]	D[K]	ϕ[-]	D[K]
293.15	7.57e+0	0.6	4.57e-1
343.15	6.79e+0	0.7	1.31e+0
393.15	6.00e+0	0.8	5.75e+0
443.15	5.20e+0	0.9	1.60e+0
493.15	4.41e+0	1.0	1.07e+1
543.15	3.65e+0	1.1	2.16e+0
593.15	2.97e+0	1.2	1.15e+1
		1.3	3.28e+0
		1.4	1.15e+1
		1.5	3.89e+0

Table 5. The error at a constant temperature, pressure and equivalence ratio is calculated according to Eq. 15.

Coefficients for the Adiabatic Flame Temperature

General Form: $T_{\text{ad}} = C_1 + C_2\phi + C_3\phi^2 + C_4\phi^3 + C_5\phi^4$

Correlation for C_i

Formulation: $C_i = C^\star_{i,1} + C^\star_{i,2}T + C^\star_{i,3}T^2 + C^\star_{i,4}T^3$

$C^\star_{1,1}$:	4.8703e+03	$C^\star_{2,1}$:	-2.0191e+04	$C^\star_{3,1}$:	3.8570e+04	$C^\star_{4,1}$:	-2.8289e+04	$C^\star_{5,1}$:	7.0777e+03
$C^\star_{1,2}$:	1.9542e−01	$C^\star_{2,2}$:	3.5862e+00	$C^\star_{3,2}$:	-7.2775e+00	$C^\star_{4,2}$:	5.5798e+00	$C^\star_{5,2}$:	-1.4609e+00
$C^\star_{1,3}$:	-9.4320e−03	$C^\star_{2,3}$:	4.2512e−02	$C^\star_{3,3}$:	-6.8629e−02	$C^\star_{4,3}$:	4.6924e−02	$C^\star_{5,3}$:	-1.1505e−02
$C^\star_{1,4}$:	5.2275e−06	$C^\star_{2,4}$:	-2.2858e−05	$C^\star_{3,4}$:	3.6164e−05	$C^\star_{4,4}$:	-2.4578e−05	$C^\star_{5,4}$:	6.0578e−06

Table 6. Coefficients of the polynomial for the adiabatic flame temperature of methane.

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III.B. ethanol

In the case of an ethanol flame, the reduced mechanism derived by Slavinskaya[17] is employed for the calculation of additional nodal points. Note, that the mechanism predicts slightly too high laminar flame speeds on the lean side, which, however, improves further towards the flammability limit.

III.B.1. Laminar Flame Speed

Figure (6) presents a comparison of the approximated laminar flame speeds with the polynomial and experimental and numerical data available in the literature. The agreement is satisfying, except in the very lean regime where the flame speed is slightly over predicted. Concerning the agreement of the polynomial with the computed nodal points no large deviations occur, see Table 7. The laminar flame speed can be reproduced for all investigated conditions with good accuracy. The corresponding coefficients are listed in Table 8.

III.B.2. Ignition Delay Time

The nodal points as the basis of the derivation of the coefficients are also computed using the mechanism established by Slavinskaya et al.[17] The observed agreement between computed values and shock tube

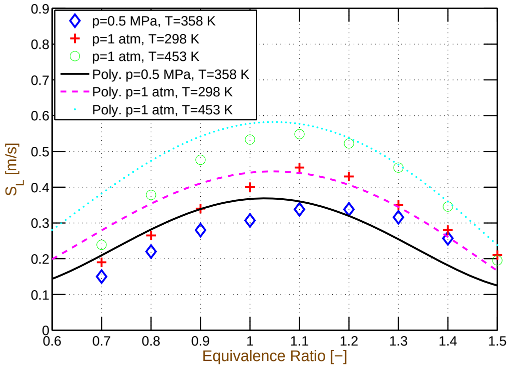

Figure 6. **Comparison of computed values by means of the polynomial with literature data. The first set of experimental values is taken from Bradley et al.[18] The second data set originates from the work of Egolfopoulos et al.[19] The last comparison includes computed data by an approximation of Liao et al.[2]**

T[K]	D[m/s]	p[bar]	D[m/s]	ϕ[-]	D[m/s]
293.15	7.72e-3	0.5	2.91e-2	0.6	1.10e-2
343.15	8.61e-3	1.0	9.27e-3	0.7	1.23e-2
393.15	1.00e-2	1.5	1.74e-2	0.8	1.20e-2
443.15	1.16e-2	2.0	1.46e-2	0.9	1.24e-2
493.15	1.30e-2	2.5	7.98e-3	1.0	1.20e-2
543.15	1.52e-2	3.0	5.99e-3	1.1	1.13e-2
593.15	1.75e-2	3.5	8.85e-3	1.2	1.23e-2
		4.0	1.12e-2	1.3	1.11e-2
		4.5	1.15e-2	1.4	1.36e-2
		5.0	7.37e-3	1.5	1.04e-2
		5.5	5.44e-3		
		6.0	1.16e-2		

Table 7. **The error at a constant temperature, pressure and equivalence ratio is calculated according to Eq. 15.**

Coefficients for the Laminar Flame Speed

General Form: $S_{\mathrm{L}} = C_1 + C_2\phi + C_3\phi^2 + C_4\phi^3 + C_5\phi^4$

Correlation for C_i

Formulation: $C_i = C^\star_{i,1} + C^\star_{i,2}T + C^\star_{i,3}T^2 + C^\star_{i,4}T^3 + C^\star_{i,5}T^4 + C^\star_{i,6}p + C^\star_{i,7}p \cdot T + C^\star_{i,8}p \cdot T^2 + C^\star_{i,9}p^2 \cdot T^2$

Note, T/300 [K], p/1e5 [Pa].

$C^\star_{1,1}$:	2.25141e+01	$C^\star_{2,1}$:	-9.14829e+01	$C^\star_{3,1}$:	1.33036e+02	$C^\star_{4,1}$:	-8.25485e+01	$C^\star_{5,1}$:	1.86148e+01
$C^\star_{1,2}$:	-6.04726e+01	$C^\star_{2,2}$:	2.43152e+02	$C^\star_{3,2}$:	-3.49015e+02	$C^\star_{4,2}$:	2.14113e+02	$C^\star_{5,2}$:	-4.78582e+01
$C^\star_{1,3}$:	6.24032e+01	$C^\star_{2,3}$:	-2.51639e+02	$C^\star_{3,3}$:	3.62718e+02	$C^\star_{4,3}$:	-2.22336e+02	$C^\star_{5,3}$:	4.94274e+01
$C^\star_{1,4}$:	-2.86708e+01	$C^\star_{2,4}$:	1.15686e+02	$C^\star_{3,4}$:	-1.66161e+02	$C^\star_{4,4}$:	1.01477e+02	$C^\star_{5,4}$:	-2.24833e+01
$C^\star_{1,5}$:	4.83125e+00	$C^\star_{2,5}$:	-1.93921e+01	$C^\star_{3,5}$:	2.77362e+01	$C^\star_{4,5}$:	-1.68625e+01	$C^\star_{5,5}$:	3.72008e+00
$C^\star_{1,6}$:	-8.14656e−01	$C^\star_{2,6}$:	3.39946e+00	$C^\star_{3,6}$:	-5.17077e+00	$C^\star_{4,6}$:	3.39903e+00	$C^\star_{5,6}$:	-8.15872e−01
$C^\star_{1,7}$:	1.47195e+00	$C^\star_{2,7}$:	-6.08923e+00	$C^\star_{3,7}$:	9.20348e+00	$C^\star_{4,7}$:	-6.10640e+00	$C^\star_{5,7}$:	1.49691e+00
$C^\star_{1,8}$:	-3.65180e−01	$C^\star_{2,8}$:	1.33738e+00	$C^\star_{3,8}$:	-2.07978e+00	$C^\star_{4,8}$:	1.41494e+00	$C^\star_{5,8}$:	-3.53490e−01
$C^\star_{1,9}$:	-1.08444e−02	$C^\star_{2,9}$:	5.94909e−02	$C^\star_{3,9}$:	-8.19545e−02	$C^\star_{4,9}$:	5.01443e−02	$C^\star_{5,9}$:	-1.16151e−02

Table 8. **Coefficients of the polynomial for the laminar flame speed of ethanol**

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experiments is of good agreement as depicted in Fig. (7), hence, providing credibility to the quality of the numerical values. The agreement between nodal points and the derived polynomial, as detailed in Table 9, is good in the entire investigated condition range. Some slightly higher relative deviations occur towards the higher temperature and pressure region, which needs to be considered. The computed coefficients are provided in Table 10.

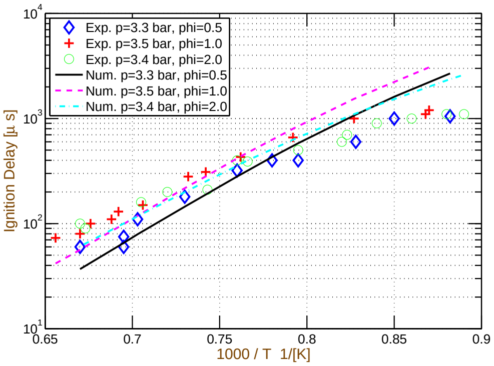

Figure 7. Comparison of the experimental data derived by Dunphy and Simmie 1991[20] with the results computed with the mechanism of Slavinskaya et al.[17] A good agreement is achieved for the investigated conditions. The mixtures correspond to 91.25 %, 95.0 % and 93.25 % dilution with Argon.

T[K]	D[s]	p[bar]	D[s]	ϕ[-]	D[s]
293.15	1.84e-6	0.5	2.29e-6	0.6	1.08e-6
343.15	2.11e-6	1.0	1.57e-6	0.7	9.47e-7
393.15	1.92e-6	1.5	1.29e-6	0.8	9.42e-7
443.15	8.35e-7	2.0	1.02e-6	0.9	9.92e-7
493.15	5.58e-7	2.5	7.10e-7	1.0	9.85e-7
543.15	5.19e-7	3.0	5.24e-7	1.1	9.64e-7
593.15	4.26e-7	3.5	4.34e-7	1.2	9.33e-7
		4.0	4.59e-7	1.3	8.60e-7
		4.5	5.54e-7	1.4	8.73e-7
		5.0	7.11e-7	1.5	9.94e-7
		5.5	8.68e-7		
		6.0	1.05e-6		

Table 9. The error at a constant temperature, pressure and equivalence ratio is calculated according to Eq. 15.

Coefficients for the Ignition Delay Time

General Form: $t_{\mathrm{i}} = C_1 + C_2\phi$

Correlation for C_i

Formulation: $C_i = C^{\star}_{i,1} + C^{\star}_{i,2} \cdot 1/T + C^{\star}_{i,3} \cdot 1/T^2 + C^{\star}_{i,4} \cdot 1/T^3 + C^{\star}_{i,5} \cdot 1/T^4 + C^{\star}_{i,6} \cdot 1/p$
$+ C^{\star}_{i,7} \cdot 1/(p \cdot T) + C^{\star}_{i,8} \cdot 1/(p \cdot T^2) + C^{\star}_{i,9} \cdot 1/(p \cdot T^3) + C^{\star}_{i,10} \cdot 1/(p \cdot T^4)$

Note, T/1000 [K], p/1e5 [Pa].

Note, coefficients are written in row formation.

$C^{\star}_{1,1}$:	2.41696e−03	$C^{\star}_{1,2}$:	-1.71533e−02	$C^{\star}_{1,3}$:	4.57797e−02	$C^{\star}_{1,4}$:	-5.45203e−02	$C^{\star}_{1,5}$:	2.44813e−02
$C^{\star}_{1,6}$:	-4.44222e−03	$C^{\star}_{1,7}$:	1.89799e−02	$C^{\star}_{1,8}$:	-2.01369e−02	$C^{\star}_{1,9}$:	-8.80977e−03	$C^{\star}_{1,10}$:	1.70852e−02
$C^{\star}_{2,1}$:	-3.92147e−03	$C^{\star}_{2,2}$:	2.47697e−02	$C^{\star}_{2,3}$:	-5.88031e−02	$C^{\star}_{2,4}$:	6.22825e−02	$C^{\star}_{2,5}$:	-2.48767e−02
$C^{\star}_{2,6}$:	5.69187e−03	$C^{\star}_{2,7}$:	-3.17361e−02	$C^{\star}_{2,8}$:	6.41149e−02	$C^{\star}_{2,9}$:	-5.47150e−02	$C^{\star}_{2,10}$:	1.61056e−02

Table 10. Coefficients of the polynomial for the ignition delay time of ethanol.

III.B.3. Adiabatic Flame Temperature

The nodal points of the adiabatic flame temperature are derived using the mechanism of Slavinskaya el al.[17] A comparison with other calculations available in the literature, see Takashi et al.[21] are in very good agreement with the approximated values by the polynomial as presented in Fig. (8). As shown in Table 11, a general good accordance between nodal values and the polynomial expression is achieved for the entire investigated range. The final polynomial coefficients are provided in Table 12.

III.C. n-decane

For the n-decane calculation of additional nodal points the reduced mechanism by Slavinskaya et al.[22] is utilised. The mechanism achieves a good agreement in terms of ignition delay times and laminar flame speeds throughout the entire investigated range.

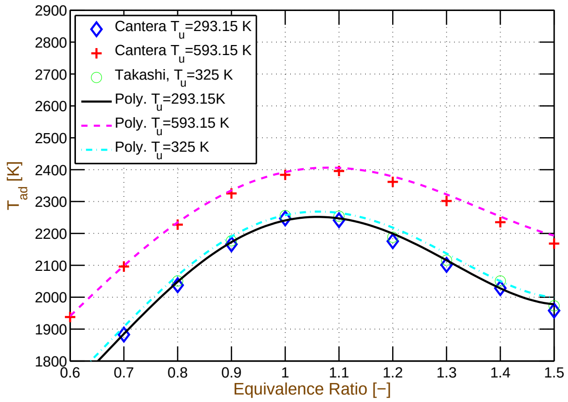

Figure 8. Comparison of polynomial approximation with the nodal values derived by Cantera for the two first data set. The third comparison is carried out with the values obtained by Takashi et al.[21]

T[K]	D[K]	ϕ[-]	D[K]
293.15	6.02e+0	0.6	4.52e-1
343.15	5.25e+0	0.7	1.55e+0
393.15	4.46e+0	0.8	3.25e+0
443.15	3.68e+0	0.9	1.23e+0
493.15	2.92e+0	1.0	6.82e+0
543.15	2.24e+0	1.1	3.56e+0
593.15	1.65e+0	1.2	7.18e+0
		1.3	2.53e+0
		1.4	9.00e+0
		1.5	1.89e+0

Table 11. The error at a constant temperature, pressure and equivalence ratio is calculated according to Eq. 15.

Coefficients for the Adiabatic Flame Temperature

General Form: $T_{\text{ad}} = C_1 + C_2\phi + C_3\phi^2 + C_4\phi^3 + C_5\phi^4$

Correlation for C_i

Formulation: $C_i = C^{\star}_{i,1} + C^{\star}_{i,2}T + C^{\star}_{i,3}T^2 + C^{\star}_{i,4}T^3$

$C^{\star}_{1,1}$:	4.2513e+03	$C^{\star}_{2,1}$:	-1.7193e+04	$C^{\star}_{3,1}$:	3.3767e+04	$C^{\star}_{4,1}$:	-2.5052e+04	$C^{\star}_{5,1}$:	6.3013e+03
$C^{\star}_{1,2}$:	4.7409e−01	$C^{\star}_{2,2}$:	2.0441e+00	$C^{\star}_{3,2}$:	-4.6865e+00	$C^{\star}_{4,2}$:	3.7163e+00	$C^{\star}_{5,2}$:	-9.8761e−01
$C^{\star}_{1,3}$:	-1.1630e−02	$C^{\star}_{2,3}$:	5.3227e−02	$C^{\star}_{3,3}$:	-8.6390e−02	$C^{\star}_{4,3}$:	5.9324e−02	$C^{\star}_{5,3}$:	-1.4585e−02
$C^{\star}_{1,4}$:	7.6668e−06	$C^{\star}_{2,4}$:	-3.4146e−05	$C^{\star}_{3,4}$:	5.4427e−05	$C^{\star}_{4,4}$:	-3.7128e−05	$C^{\star}_{5,4}$:	9.1518e−06

Table 12. Coefficients of the polynomial for the adiabatic flame temperature of ethanol.

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III.C.1. Laminar Flame Speed

Figure (9) contains a comparison of two different conditions for the laminar flame speed computed with the polynomial and experimental data. The agreement in both cases is satisfying. Moreover, no large deviations occur between the nodal values and the polynomial as shown in Table 13. The laminar flame speed can be reproduced for all investigated conditions with good accuracy. The corresponding coefficients are listed in Table 14.

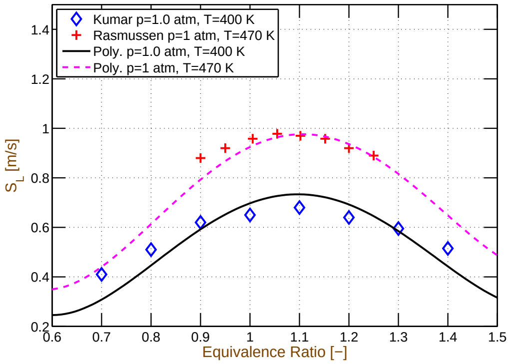

Figure 9. Comparison of computed values by means of the polynomial with literature data. The first set of experimental values is taken from Kumar et al.[23] The second data set originates from the work of Skjoth-Rasmussen et al.[24]

T[K]	Error	p[bar]	Error	ϕ[-]	Error
293.15	1.80e-2	0.5	2.21e-2	0.6	2.59e-2
343.15	2.16e-2	1.0	2.96e-2	0.7	3.45e-2
393.15	2.56e-2	1.5	3.55e-2	0.8	1.47e-2
443.15	3.02e-2	2.0	3.52e-2	0.9	4.80e-2
493.15	3.48e-2	2.5	3.28e-2	1.0	3.42e-2
543.15	3.96e-2	3.0	3.09e-2	1.1	4.03e-2
593.15	4.60e-2	3.5	2.92e-2	1.2	1.83e-2
		4.0	2.74e-2	1.3	3.91e-2
		4.5	2.56e-2	1.4	3.46e-2
		5.0	2.73e-2	1.5	1.73e-2
		5.5	3.33e-2		
		6.0	4.05e-2		

Table 13. The error at a constant temperature, pressure and equivalence ratio is calculated according to Eq. 15.

Coefficients for the Laminar Flame Speed

General Form: $S_{\mathrm{L}} = C_1 + C_2\phi + C_3\phi^2 + C_4\phi^3 + C_5\phi^4$

Correlation for C_i

Formulation: $C_i = C^\star_{i,1} + C^\star_{i,2}T + C^\star_{i,3}T^2 + C^\star_{i,4}T^3 + C^\star_{i,5}T^4 + C^\star_{i,6}p + C^\star_{i,7}p \cdot T + C^\star_{i,8}p \cdot T^2 + C^\star_{i,9}p^2 \cdot T^2$

Note, T/300 [K], p/1e5 [Pa].

$C^\star_{1,1}$:	-6.09241e+01	$C^\star_{2,1}$:	2.60205e+02	$C^\star_{3,1}$:	-4.01296e+02	$C^\star_{4,1}$:	2.64740e+02	$C^\star_{5,1}$:	-6.32998e+01
$C^\star_{1,2}$:	1.86125e+02	$C^\star_{2,2}$:	-7.96783e+02	$C^\star_{3,2}$:	1.23133e+03	$C^\star_{4,2}$:	-8.12882e+02	$C^\star_{5,2}$:	1.94284e+02
$C^\star_{1,3}$:	-1.94090e+02	$C^\star_{2,3}$:	8.30943e+02	$C^\star_{3,3}$:	-1.28441e+03	$C^\star_{4,3}$:	8.49108e+02	$C^\star_{5,3}$:	-2.03377e+02
$C^\star_{1,4}$:	9.00070e+01	$C^\star_{2,4}$:	-3.86284e+02	$C^\star_{3,4}$:	5.98929e+02	$C^\star_{4,4}$:	-3.96813e+02	$C^\star_{5,4}$:	9.51801e+01
$C^\star_{1,5}$:	-1.56202e+01	$C^\star_{2,5}$:	6.72893e+01	$C^\star_{3,5}$:	-1.04651e+02	$C^\star_{4,5}$:	6.95071e+01	$C^\star_{5,5}$:	-1.67020e+01
$C^\star_{1,6}$:	1.35767e+00	$C^\star_{2,6}$:	-5.62723e+00	$C^\star_{3,6}$:	8.51518e+00	$C^\star_{4,6}$:	-5.58263e+00	$C^\star_{5,6}$:	1.33465e+00
$C^\star_{1,7}$:	-2.07916e+00	$C^\star_{2,7}$:	8.79306e+00	$C^\star_{3,7}$:	-1.34222e+01	$C^\star_{4,7}$:	8.73566e+00	$C^\star_{5,7}$:	-2.05006e+00
$C^\star_{1,8}$:	1.89322e+00	$C^\star_{2,8}$:	-7.95661e+00	$C^\star_{3,8}$:	1.16756e+01	$C^\star_{4,8}$:	-7.30360e+00	$C^\star_{5,8}$:	1.65391e+00
$C^\star_{1,9}$:	-1.99070e−01	$C^\star_{2,9}$:	8.24998e−01	$C^\star_{3,9}$:	-1.18174e+00	$C^\star_{4,9}$:	7.16808e−01	$C^\star_{5,9}$:	-1.57116e−01

Table 14. Coefficients of the polynomial for the laminar flame speed of n-decane

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III.C.2. Ignition Delay Time

The nodal points as the basis of the derivation of the coefficients are also computed employing the mechanism proposed by Slavinskaya et al.[22] The observed agreement between computed values and shock tube experiments is of good agreement as depicted in Fig. (10), hence, providing credibility to the quality of the nodal points. The agreement between nodal points and the derived polynomial, as detailed in Table 15, exhibits large relative deviations. This is mitigated by the absolute values, see Table 15. As n-decane has the nature of igniting very quickly, the ignition delay times in the high temperature zone (˜1800K) are of very small magnitude, hence, not representing a large weight to the least squares method. Consequently, at high temperatures, although the deviations is of only tenth of μs, they represent a relative error of sometimes 100%, whereas the least squares method optimizes the function for large ignition delay times where the occurring absolute differences can be of several orders larger. In summary, the values in the high temperature zones are not useful for a comparison with experimental data. On the contrary, for a numerical simulation, where the simulation time is mostly of larger order than one μs ignition delay time predicted by the polynomial in the high temperature region is exceeded within one time step, which provides a sufficient accuracy. The computed coefficients are given in Table 16.

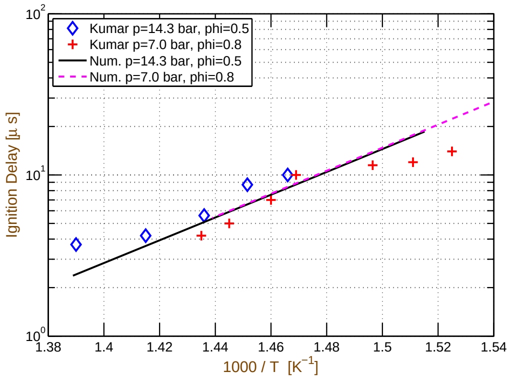

Figure 10. Comparison of the experimental data derived by Kumar et al.[25] with the nodal points computed with the mechanism of Slavinskaya et al.[17] A good agreement is achieved for the investigated conditions.

T[K]	D[s]	p[bar]	D[s]	ϕ[-]	D[s]
293.15	6.27e-6	0.5	1.01e-5	0.6	5.22e-6
343.15	3.12e-6	1.0	5.31e-6	0.7	3.22e-6
393.15	3.84e-6	1.5	4.31e-6	0.8	3.08e-6
443.15	2.30e-6	2.0	2.77e-6	0.9	3.50e-6
493.15	1.86e-6	2.5	2.22e-6	1.0	3.44e-6
543.15	2.10e-6	3.0	1.92e-6	1.1	2.89e-6
593.15	2.46e-6	3.5	1.64e-6	1.2	2.38e-6
		4.0	1.51e-6	1.3	1.60e-6
		4.5	1.44e-6	1.4	1.71e-6
		5.0	1.40e-6	1.5	2.55e-6
		5.5	1.42e-6		
		6.0	1.41e-6		

Table 15. The error at a constant temperature, pressure and equivalence ratio is calculated according to Eq. 15.

Coefficients for the Ignition Delay Time

General Form: $t_{\mathrm{i}} = C_1 + C_2\phi$

Correlation for C_i

Formulation: $C_i = C^\star_{i,1} + C^\star_{i,2} \cdot 1/T + C^\star_{i,3} \cdot 1/T^2 + C^\star_{i,4} \cdot 1/T^3 + C^\star_{i,5} \cdot 1/T^4 + C^\star_{i,6} \cdot 1/p$
$+ C^\star_{i,7} \cdot 1/(p \cdot T) + C^\star_{i,8} \cdot 1/(p \cdot T^2) + C^\star_{i,9} \cdot 1/(p \cdot T^3) + C^\star_{i,10} \cdot 1/(p \cdot T^4)$

Note, T/1000 [K], p/1e5 [Pa].

Note, coefficients are written in row formation.

$C^\star_{1,1}$:	5.41490e−02	$C^\star_{1,2}$:	-3.44915e−01	$C^\star_{1,3}$:	8.21339e−01	$C^\star_{1,4}$:	-8.67036e−01	$C^\star_{1,5}$:	3.42581e−01
$C^\star_{1,6}$:	-4.84663e−02	$C^\star_{1,7}$:	2.82626e−01	$C^\star_{1,8}$:	-6.05832e−01	$C^\star_{1,9}$:	5.61393e−01	$C^\star_{1,10}$:	-1.87151e−01
$C^\star_{2,1}$:	-6.57936e−02	$C^\star_{2,2}$:	4.16056e−01	$C^\star_{2,3}$:	-9.83080e−01	$C^\star_{2,4}$:	1.02895e+00	$C^\star_{2,5}$:	-4.02643e−01
$C^\star_{2,6}$:	7.31715e−02	$C^\star_{2,7}$:	-4.47257e−01	$C^\star_{2,8}$:	1.01743e+00	$C^\star_{2,9}$:	-1.01960e+00	$C^\star_{2,10}$:	3.79219e−01

Table 16. Coefficients of the polynomial for the ignition delay time of n-decane.

III.C.3. Adiabatic Flame Temperature

The nodal points of the adiabatic flame temperature are derived using the skeletal mechanism of Slavinskaya el al.[17] for n-decane. As no literature data could be found regarding the adiabatic flame temperature of n-decane, a comparison with other sources cannot be presented. However, the excellent agreement of the polynomials for the adiabatic flame temperature of methane and ethanol with various studies provide credibility to the computed nodal points. As shown in Fig. (11) and as detailed in Table 17, a general good accordance between nodal values and the polynomial expression is achieved for the entire investigated range. The final polynomial coefficients are provided in Table 18.

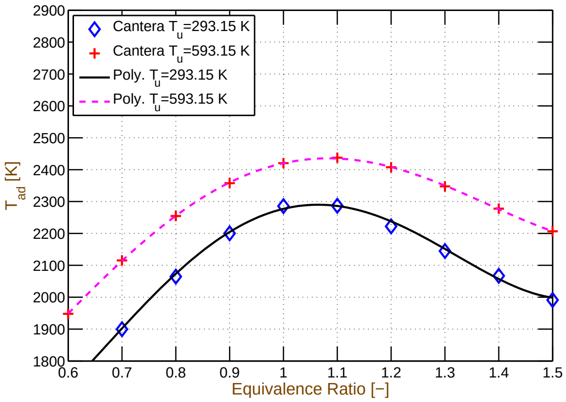

Figure 11. Comparison of polynomial approximation with the nodal values derived by Cantera for two different sets of temperature. A very satisfying agreement is achieved by the polynomial.

T[K]	D[K]	ϕ[-]	D[K]
293.15	5.66e+0	0.6	4.08e-1
343.15	4.82e+0	0.7	1.19e+0
393.15	3.99e+0	0.8	2.97e+0
443.15	3.22e+0	0.9	1.69e+0
493.15	2.51e+0	1.0	4.81e+0
543.15	1.88e+0	1.1	3.32e+0
593.15	1.33e+0	1.2	6.33e+0
		1.3	3.24e+0
		1.4	7.32e+0
		1.5	2.16e+0

Table 17. The error at a constant temperature, pressure and equivalence ratio is calculated according to Eq. 15.

Coefficients for the Adiabatic Flame Temperature

General Form: $T_{\text{ad}} = C_1 + C_2\phi + C_3\phi^2 + C_4\phi^3 + C_5\phi^4$

Correlation for C_i

Formulation: $C_i = C^{\star}_{i,1} + C^{\star}_{i,2}T + C^{\star}_{i,3}T^2 + C^{\star}_{i,4}T^3$

$C^{\star}_{1,1}$:	4.5619e+03	$C^{\star}_{2,1}$:	-1.8797e+04	$C^{\star}_{3,1}$:	3.6565e+04	$C^{\star}_{4,1}$:	-2.6974e+04	$C^{\star}_{5,1}$:	6.7575e+03
$C^{\star}_{1,2}$:	-5.4783e−01	$C^{\star}_{2,2}$:	6.8616e+00	$C^{\star}_{3,2}$:	-1.2524e+01	$C^{\star}_{4,2}$:	9.1129e+00	$C^{\star}_{5,2}$:	-2.3187e+00
$C^{\star}_{1,3}$:	-1.1823e−02	$C^{\star}_{2,3}$:	5.3779e−02	$C^{\star}_{3,3}$:	-8.7093e−02	$C^{\star}_{4,3}$:	5.9618e−02	$C^{\star}_{5,3}$:	-1.4601e−02
$C^{\star}_{1,4}$:	8.6544e−06	$C^{\star}_{2,4}$:	-3.8317e−05	$C^{\star}_{3,4}$:	6.0911e−05	$C^{\star}_{4,4}$:	-4.1390e−05	$C^{\star}_{5,4}$:	1.0154e−05

Table 18. Coefficients of the polynomial for the adiabatic flame temperature of n-decane.

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IV. Conclusion

For three fuels and three characterizing flame properties, functional correlations have been derived, offering an alternative to tabulated values in simplified chemistry models. Especially, the handling and implementation of simplified chemistry models can be further eased, when the task reduces to the inclusion of an algebraic expression. Furthermore, the polynomials may be of service, when a a short glance at one property for a certain set of conditions is required. Regarding the overall quality of the derived approximation, the agreement of the polynomial in terms of the laminar flame speed with experimental data sets is satisfying. In the case of ethanol some larger deviations occur for the laminar flame speed in the lean - very lean region. The laminar flame speed for methane and n-decane has been matched accurately by the polynomial for the entire envisaged range. In the case of the ignition delay time, a comparison of the derived polynomial with experimental data is impeded by the lack of sufficient experimental data. Hence, the quality of the computed nodal points is demonstrated for mostly diluted mixtures for which a large data basis is available. The accuracy is very satisfying providing credibility to the obtained polynomial by the good agreement of the nodal values. Considering the adiabatic flame temperature, the validation in the case of methane is accomplished with available values from the literature, which shows a very good agreement. For ethanol the polynomial could be matched with experimental data as well, demonstrating a very satisfying accuracy. Solely, for n-decane no literature data is avaliable for an accurate comparison. However, the values computed with Cantera, which for the other fuels, provided an excellent data base were compared with the polynomial, pointing out the quality of the chosen functional form.

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