

## ADAPTATION OF N-HEPTANE AUTOIGNITION TABULATION FOR COMPLEX CHEMISTRY MECHANISMS

by

**Marko BAN<sup>\*</sup> and Neven DUIĆ**

Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia

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*The adaptation of auto-ignition tabulation for effective use of complex chemical mechanisms will be presented in this paper. Taking cool flame ignition phenomenon into account could improve numerical simulations of combustion in compression ignition engines. Current approaches of successful simulation of this phenomenon are based on the extraction of ignition delay times, heat releases and also reaction rates from tabulated data dependant on four parameters: temperature, pressure, equivalence ratio, and exhaust gasses mass fraction.*

*The methods described here were used to create lookup tables including cool flame using a comprehensive chemical mechanism without including reaction rates data (as used by other authors). The method proved to be stable for creating tables and these results will be shown, as well as initial implementation results using the tables in computational fluid dynamics software.*

*Key words: auto-ignition, tabulation, n-heptane, ECFM-3Z, comprehensive mechanisms*

### Introduction

Recent rapid advances in computer power lead to increased use of computational tools in engine design, significantly reducing the costs of simulations in comparison to engine experiments. Also, more stringent pollutant emissions' regulations force combustion chamber designers to develop new approaches to satisfy all the necessary requirements [1-3]. Thus, there has been significant improvement in the physical sub models used in engine simulations, and the enhanced accuracy as made the use of computational tools advantageous for generating a better understanding of the transient physical and chemical phenomena that occur in internal combustion engines. The goal of this study was to improve the prediction of diesel fuel autoignition processes in the computational fluid dynamics (CFD) code called „FIRE” using the extended coherent flame model with three zone approach (ECFM-3Z) [4].

Flame development, power output and emissions formation are determined by the process of autoignition in diesel IC engines which is dependent on chemical and physical processes. The first kinds of processes are pre-combustion reaction of the fuel with air and residual gases, high temperature combustion and emissions formation. The main physical processes include at-

<sup>\*</sup> Corresponding author; e-mail: marko.ban@fsb.hr

omization of liquid fuel, evaporation of fuel droplets, and turbulent mixing of vapor with air. Rather than trying to simulate the complex behavior of diesel fuel itself the replacement fuel of choice is n-heptane due to its cetane number of approximately 56, which is similar to that of ordinary diesel fuel.

Current diesel (n-heptane) autoignition model included in CFD code "FIRE" used a tabulated data acquired by running 0-D calculations varying following initial parameters: temperature, pressure, equivalence ratio, and exhaust gas recirculation (EGR) mass fraction [5]. These values were used to simulate the exact ignition moment using a precursor variable, as explained in detail later in the paper. However, existing data provides only the main ignition delays, which is sometimes not accurate enough without taking cool flame phenomenon into account *e. g.* when running simulations in a low temperature region.

During the work described in this paper, the oxidation process of auto-ignition is calculated using CHEMKIN II code, assuming zero dimension and adiabatic conditions. Initial calculations were performed using three levels of chemical model complexity to select an optimal chemical mechanism regarding calculation time and accuracy.

### Chemistry background and numerical approach

When studying the complex chemical mechanism, it is possible to get a comprehensive insight of the chemical kinetics behind the phenomena of auto ignition. Skeletal mechanism (that include the main species and reactions) consist in general of 20-80 species with less than 250 reactions [6, 7]. These can further be simplified to 4-40 steps, but this approach (done by mathematical transformations) can cause the loss of physical meaning of the individual species [8]. The complete complex reaction mechanism for n-heptane oxidation includes 2450 elementary reactions with 550 chemical species. The detailed n-heptane mechanism [9] is intended to cover the entire range of conditions from low-temperature (600-900 K) pyrolysis and oxidation to high-temperature combustion. Several methods are used to reduce the chemical mechanisms to the size appropriate for reasonable computation (skeletal or reduced models) based on sensitivity analysis, and others (the quasi-steady-state assumption, the intrinsic low-dimensional manifold approach, or the computational singular perturbation method) [10, 11]. Also, one could base the survey on whether the mechanism simplification method is based on reduction of reactions [12] or reduction of species [13, 14]. Principally, one can state that full, complex models are validated with experimental data, while the reduction is made against the full mechanism calculation results of the interest (flame speed, auto-ignition) [15-17].

Recent studies show that, using auto-ignition delay as an optimization criterion, the above-mentioned detailed mechanism could be reduced to 170-180 species [11], and some show improvement using even more reduced mechanisms (67 species and 265 reactions [18]). More useful information about this topic could be found in [19-21].

Cool flame phenomenon is especially important associated with knocking and homogeneous charge compression ignition combustion in internal combustion engines, and refers to the low-temperature (500-800 K) chemical activity partially oxidizing the hydrocarbon fuel without burning it completely (with no formation of soot precursors). Also, a characteristic negative temperature coefficient of reaction rate is associated with this phenomenon, due to the competition between chain-termination and chain branching reactions [22]. Special case is so called oscillatory cool flames, which are getting more attention recently [23]. Since they include

specific interaction of thermal and chemical feedback they will not be studied further in this paper.

N-heptane, which is a straight-chained fuel, is assumed to lead to alkenyl decomposition products with alkyl radical and olefins.

Due to the comprehensive mechanism of n-heptane oxidation, n-heptane molecules undergo H-atom abstraction at high and low temperatures, leading to the formation of structurally distinct alkyl radicals. When alkane fuels have to stay partially or fully premixed in an oxidizing atmosphere at elevated temperatures and pressures, ignition can occur in a multistage mode. The ignition process can follow completely different schemes of oxidation and is controlled by two different chain-branching reaction mechanisms: the low-temperature reaction path, where the fuel is oxidized by O<sub>2</sub> in degenerated branched chains, and the high-temperature path, where the fuel is rapidly oxidized into C<sub>2</sub> and C<sub>1</sub> hydrocarbons and subsequently consumed. The low-temperature branch is quite complex and proceeds via different sub mechanisms, which are sensitively controlled by the temperature [9].

At high temperatures, reaction propagates via radical β-scission, the initial step in the chemistry of thermal cracking of hydrocarbons and the formation of free radicals. They are formed upon splitting the carbon-carbon bond. Free radicals are extremely reactive and short-lived. When a free radical undergoes a β-scission, the free radical breaks two carbons away from the charged carbon producing an olefin and a primary free radical, which has two fewer carbon atoms. At low and intermediate temperatures (600-900 K), peroxide chemistry becomes more important. The n-heptyl radical reacts with molecular oxygen, R + O<sub>2</sub> = RO<sub>2</sub>, forming a heptylperoxy radical (C<sub>7</sub>H<sub>15</sub>OO). After the internal H-abstraction, the radical undergoes a second addition of O<sub>2</sub> forming hydroperoxy-heptylperoxy radicals, which are very unstable and decompose easily. Its products are both chain propagating and degenerating branching agents [9].

In this study of auto-ignition phenomenon, a FORTRAN subroutine library CHEMKIN II was used, assuming zero dimension and adiabatic changes. It is generally used to predict the time-dependent kinetics behavior of a homogenous gas mixture in a closed system. There are many possibilities for the chemical kinetics problems that one may need to solve for various applications [24, 25]. The problems interesting to this study are:

- an adiabatic system with constant pressure, and
- an adiabatic system with constant volume.

The energy equation for the constant volume case is:

$$c_v \frac{dT}{dt} - \sum_{k=1}^K h_k \dot{\omega}_k W_k = 0 \quad (1)$$

where the mean specific heat of the mixture is represented by  $c_v$ . The net chemical production rate  $\dot{\omega}_k$  of each species results from a competition between all the chemical reactions involving that species. Each reaction proceeds according to the law of mass action and the forward rate coefficients are in the modified Arrhenius form [24].

$$k_f = AT^\beta \exp \left( \frac{-E}{RT} \right) \quad (2)$$

where the activation energy  $E$ , the temperature exponent  $\beta$ , and the pre-exponential constant  $A$  represent the parameters in the model formulation.

Since monitoring the cool flame phenomenon was one of the main topics of this work, a generalized routine to “catch” both cool flame and main ignition had to be developed. A useful basic definition of the ignition delay time was obtained from [26] which states that it could be presented as the time at which the temperature theoretically becomes infinite (the asymptote of the temperature curve).

Also, some other criteria had to be implemented in the code to make it possible to get both the cool flame and main ignition delay times, as well as to filter out the misleading ignition candidates at the beginning of the calculation and around 1000 K. First approach was to use the temperature gradient which is tested at each time step according to eq. (3) and if an inflexion occurred the time is stored into a vector variable:

$$\text{sign} \frac{d^2T}{dt^2} \Big|_t \quad \text{sign} \frac{d^2T}{dt^2} \Big|_{t \text{ dt}} \quad (3)$$

If there is only one record in the vector variable at the end of the calculation, no cool flame ignition had occurred. In other case the first record is taken to be the cool flame ignition delay, and the last one is taken as main ignition delay. This approach provides good general and robust way to test the ignition delay at real time but provides a problem when implementing in ECFM-3Z (discussed later).

Second approach is also commonly used, and assumes fixed temperature increase as an ignition criterion. In this study combination of both approaches is used with first ignition occurring when temperature increases by 10 degrees, after which the ignition tracer is reset at the temperature inflexion point. From this point forward the second ignition catching criteria is waiting for the temperature increase of 30 degrees.

After modeling the tabulation, the next step was the implementation of the tabulated data into the CFD solver. Generally speaking, as far as the combustion modeling is concerned, presumed conditional moment (PCM) approach, as well as recently developed diffusion-flame PCM (DF-PCM) presents a simplified version of conditional moment closure (CMC) approach, where one assumes conditional moment of a reaction progress variable and the reaction rates are supplied by a database created for premixed and non-premixed stationary flamelets [27, 28]. As a last modeling approach taken into the consideration here is the (ECFM-3Z) model which assumes two zones of burned-unburned and three zones of mixing (pure air, pure fuel, and completely mixed zone), enabling a good qualitative description of autoignition, propagating, and diffusion flame.

In the ECFM-3Z combustion model, used in this work, the ignition delay is computed either through a correlation or through an interpolation from tabulated values (the latter method is the one of the interest for this work) [29, 32]. An intermediate species integrates the advance in the auto-ignition process for each time step in each computational grid cell (dependent on the cell's current pressure, temperature, and mixture composition). When the delay time is reached, the mixed fuel is oxidized with a chemical characteristic time.

Source term of the intermediate species is as [5, 30, 32]:

$$\frac{\partial \bar{N}_I^M}{\partial t} = \bar{N}_{TFu}^M \Big|_M F(\tau_d) \quad (4)$$

where M denotes the mixture zone, represents fuel tracer in the mixture zone, and  $F$  is a function of delay time (tabulated value) [15][30]:

$$F(\tau_d) = \frac{\sqrt{B^2 \tau_d^2 - 4(1 - B\tau_\delta) \frac{N_I^M}{N_{TFu}^M}}}{\tau_d} \quad (5)$$

where  $B$  is a constant set to 1 s.

The same approach is used in modeling the cool flame ignition according to [30]. In this case if the intermediate species reach the tabulated value for cool flame delay (first combustion stage occurs), only a part of fuel should be consumed. This part is calculated as a ratio of two more tabulated values, cool flame and main ignition heat release. This approach is still an issue open to further discussion, but the results with the current setup seem very promising. Original authors of this cool flame ignition calculation approach additionally suggest the tabulation of reaction rates for more correct cool flame representation [32]. However, the results of this paper show that not including the reaction rates in the tabulation and later use of those is not really needed for providing temperature field of good quality.

Representation of this methodology is clearly visible in fig. 1 where one can see the evolution of cool flame precursor (CF PREC) and main ignition precursor (M.IGN. PREC) against the temperature (TEMP) and fuel tracer variable (FU TRACER).

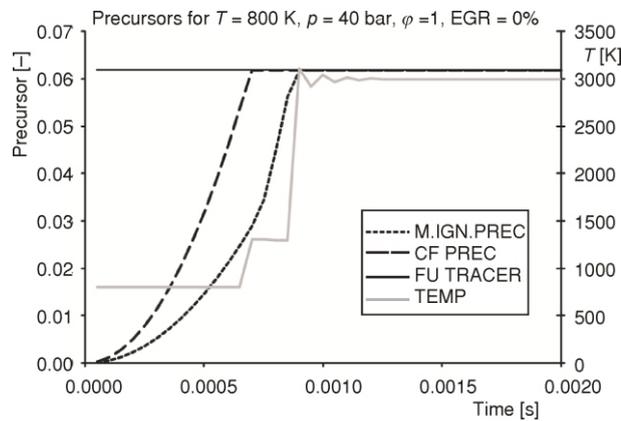


Figure 1. Ignition precursors in the ECFM-3Z model

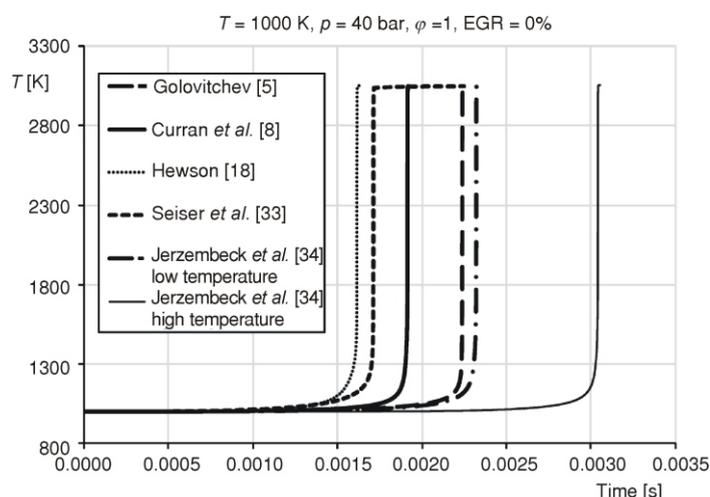
## Tabulation

The ignition data tables should provide the following data: cool flame ignition delay, cool flame heat release, main ignition delay, and main heat release. Initial parameter ranges were taken out of existing tables (consisting of only main ignition delay times) and count in total 8640 points which would present a great amount of strain to the available computer power when using a mechanism of greater degree of complexity. Therefore, the right ratio of necessary computer power and mechanism accuracy had to be taken into consideration.

Out of publically available n-heptane mechanisms [6, 9, 17, 18, 33, 34] (compared in fig. 2) three different chemical mechanisms have been closely compared on more calculation points:

- simple Golovitchev with 59 species and 291 reactions [6] (simple in further text),
- reduced Seiser *et al.* with 159 species, 770 reactions [33] (LLNL reduced in further text), and
- detailed Curran *et al.* with 556 species, 2540 reactions [9] (LLNL complex in further text).

Closer comparison of the mechanisms show that the LLNL reduced mechanism clearly agrees more with the complex one than the simple mechanism which, in most cases, provides under-prediction of the ignition delays. Since the complex mechanism would be to demanding computational time – wise, the reduced mechanism was chosen for final table.



**Figure 2. Comparison of available n-heptane mechanisms using CHEMKIN package for a single set of initial conditions**

data points would be below 3000. Simple mechanism calculations were performed to show dependence of ignition delay time on initial pressure and temperature, as well as the influence of EGR ratio. For initial temperatures of over 800 K cool flame ignition was either very hard to detect or so close to the main ignition that there was no need to separate the two. The results also suggest that there was room for coarser distribution of temperature and pressure, *e. g.* no need for any temperature distribution points between 1100 K and 1500 K, or changing the distribution from 20 K to 40 K in the lower part of the temperature distribution. Coarse distribution has also shown the characteristic wave-like dependence in the low temperature area, and has reduced the number of calculations to about 2500. This is well inside the needed number of calculations but looking at the cool flame ignition delays, there was still a demand to leave the initial temperatures with finer distribution in the 600-750 K temperature region. On the other hand, when looking at the pressure dependencies one can easily come to conclusion that there is no special need for all the pressure points on the high pressure side (above 40 bar), thus compensating for finer low temperature distribution. The data shown in tab. 1 is the final table done with several refinements (two more points for pressure and one more point for equivalence ratio were added) finally lowering the needed amount of calculation points to around 1800.

The recirculation exhaust gas is represented as the idealized products of a complete combustion – it comprises  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{O}_2$ , and  $\text{N}_2$ .

**Table 1. Initial data for n-heptane tabulation using LLNL Curran reduced mechanism**

Temperature [K]	600-750 K (20 K step), 790-1110 K (40 K), and 1500 K						
Pressure [bar]	10	20	30	40	50	60	80
Equivalence ratio [-]	0.3	0.5	0.7	1	1.5	3	
EGR [-]	0	0.3	0.6	0.8			

The approach to initially use a simpler mechanism for definition of possible distribution ranges fit for coarsening was adopted. The idea behind this way of data investigation is to find the areas of linear (or near-linear) dependence of ignition delays on temperature and pressure to reduce the number of necessary calculations. Using the LLNL reduced mechanism (agreed on the fact that results it provides are close enough to the LLNL complex mechanism which was set as a reference one), acceptable number of

The data is stored as ASCII values making it very easy to manipulate and refine before importing in the CFD code.

Using the Golovitchev [6] and LLNL reduced mechanism [33], the result showed improvement regarding higher ignition delay times as seen in figs. 3 and 4.

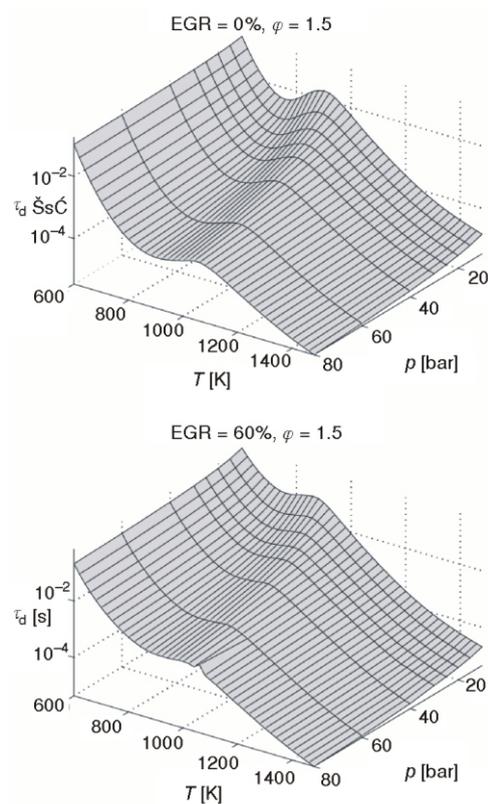


Figure 3. Interpolation table with Golovitchev mechanism [6]

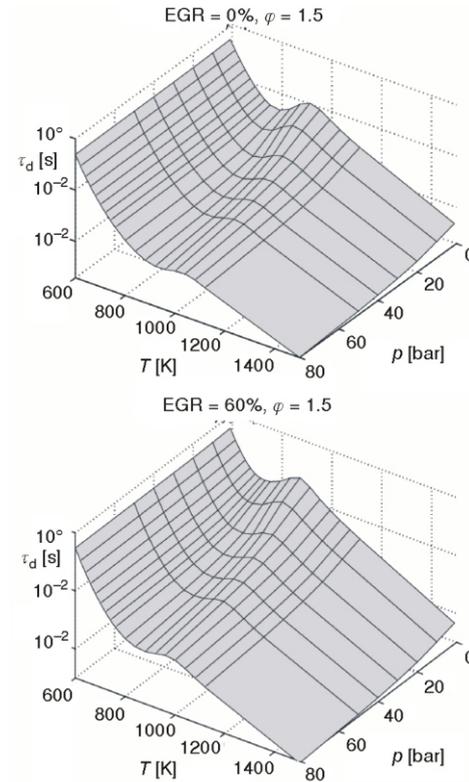
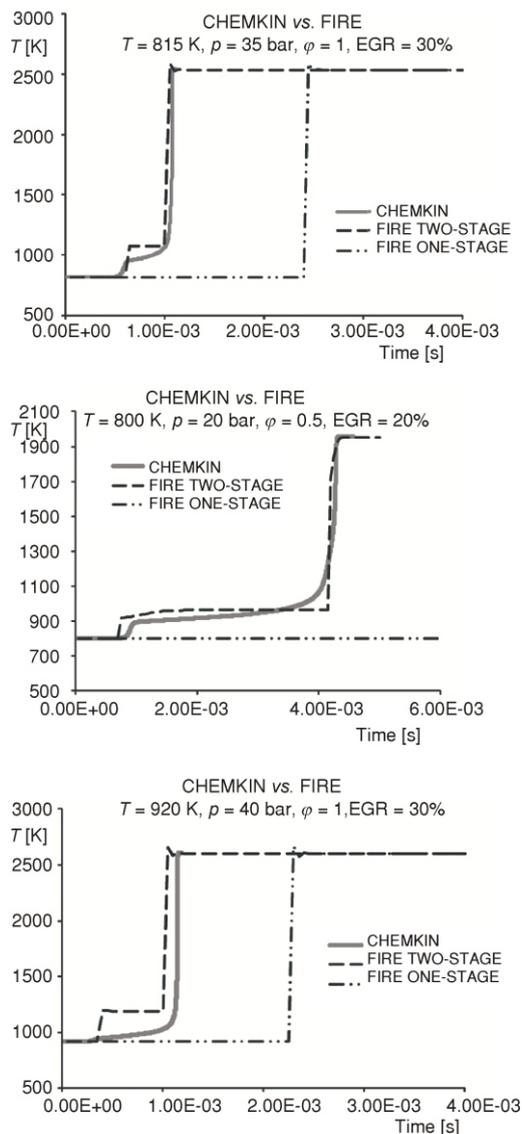


Figure 4. Interpolation table using reduced LLNL mechanism [33]

### CFD simulation results and discussion

After the data had been imported as a database into FIRE software, and ECFM-3Z ignition module modified to use it using the software's user function capabilities [4, 35], a simple calculation case has been set up to try and recreate the CHEMKIN calculation results using ECFM-3Z combustion model. The calculation domain set up included quasi-2-D, constant volume with no heat flux through the walls, and used the ECFM-3Z combustion model with modified two-stage ignition.

On fig. 5 comparison results for three selected initial data combinations varying temperature, pressure, equivalence ratio, and EGR mass fraction are shown. The data selected represent various cases with smaller and larger deviations in values from the ones used to make the database, to check for any major issues with interpolation methodology. Selected sets of results



**Figure 5. Simulation results comparing new two-stage ignition model (FIRE TWO-STAGE) and existing one stage**

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show good agreement between the CHEMKIN calculated values, and the results obtained using FIRE solver with ignition model described in this paper (FIRE TWO-STAGE). Also, results obtained using ECFM-3Z model with previously implemented one-stage ignition are included (FIRE ONE-STAGE), clearly showing the improvement using the new ignition model.

Last part of the figure also shows the importance of the second ignition criterion (fixed temperature increase), because if inflexion criteria is used one gets later ignition times since it occurs at around 50% of the final temperature. Since the ignition delay time is used in ECFM-3Z model as an ignition start trigger, this yields the late ignition in some cases (with steeper temperature gradients).

The approach of using released heat for cool and main ignition for calculating the fuel consumption at cool flame ignition remains open to further investigation since it provides slight over-prediction in terms of cool flame temperature in some cases.

### Conclusions

The overall approach proved itself to be reliable, robust for calculation and easy for post-processing and data manipulation. There was successful attempt to use other mechanisms and fuels using the tabulation application (methane, ethanol, DME, iso-octane), making it a promising tool for future use in ignition simulations on a wider scope.

Presented methodology for including low temperature ignition in CFD environment provided good agreement with 0-D chemistry calculations, proving that for this type of application there is no need for adding more information into the database (reaction rates).

## Nomenclature

$A$  – pre-exponential constant, [–]  
 $B$  – constant, [s]  
 $c_v$  – specific heat capacity at constant volume, [Jkg<sup>-1</sup>K<sup>-1</sup>]  
 $E$  – activation energy, [Jmol<sup>-1</sup>]  
 $F$  – function, [–]  
 $h$  – specific enthalpy, [Jkg<sup>-1</sup>]  
 $k$  – forw./rev. rate constant, [–]  
 $N$  – tracer, [–]  
 $R$  – universal gas constant, [Jmol<sup>-1</sup>K<sup>-1</sup>]  
 $T$  – mixture temperature, [K]  
 $W$  – molar weight, [kgmol<sup>-1</sup>]

### Greek letters

$\beta$  – temperature exponent, [–]

– specific volume, [m<sup>3</sup>kg<sup>-1</sup>]  
 $\dot{\omega}$  – chemical production rate, [molm<sup>-3</sup>s<sup>-1</sup>]  
 $\tau$  – time, [s]

### Subscripts and superscripts

d – delay (ignition)  
I – intermediate species  
k – species index  
M – mixture zone  
TFu – fuel

### Acronyms

EGR – exhaust gas recirculation  
LLNR – Lawrence Livermore National Laboratory, Livermore, Cal., USA

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