

Analysis of Thermodynamic Characteristics of Diesel Engine Emission Control Strategies Using a Multi-Zone Combustion Model

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ABSTRACT

The paper describes a zero-dimensional crank angle resolved combustion model which was developed for the analysis and prediction of combustion in compression ignition (CI) engines. The model relies on the multi zone combustion model (MZCM) approach of Hiroyasu. The main sub-models were taken from literature and extended with additional features described in this paper.

A special procedure described in a previous paper is used to identify the mechanisms of the combustion process on the basis of the measured cylinder pressure trace. Based on the identified mechanisms the present work concentrates on the analysis of the causal effects that predominantly control the combustion process and the formation of NO_x and Soot. The focus lies on the changes of the thermodynamic states and the composition of the reaction zones caused by different emission control strategies.

Finally this knowledge is applied to predict the characteristics of cycle related data such as thermal efficiency, process temperatures, pressures and combustion emissions as function of changes in engine settings. Based on this data procedures for minimization of fuel consumption and emissions are discussed.

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INTRODUCTION

A profound knowledge of combustion characteristics is essential for the development of control strategies of diesel engines. For this purpose combustion models are usually applied which predict engine performance and the formation of emissions by adequate modeling approaches. However, models considerably differ in complexity and accuracy. Zero-dimensional, crank angle resolved cylinder models are commonly applied as they provide a high content of information within short computational time. The multi-zone combustion model (MZCM) that is used in this work was introduced and discussed in detail in [22]. It follows the basic principle of the Hiroyasu Spray Model [4] which has been widely used in the literature, e.g. [2, 5, 6].

To compensate for the fact that the MZCM does not imply spatial information of the combustion chamber, the inhomogeneous spreading of chemical reactions in the

combustion chamber is approximated by breaking down the cylinder volume into chemical reaction zones. Each of these zones has its own history of thermodynamic state and composition. The heat release is calculated within the individual zones by an Arrhenius type approach. Within each zone the supply of fuel and oxygen to chemical reactions considers fuel evaporation and the charge entrainment mechanism into the fuel spray. In this way the entire combustion process in the cylinder of an engine is composed of a diverse variety of sub-reactions.

The previous publication [22] identified the most important model parameters using performance and emission measurements of three different engines at various operating points. It was demonstrated that the model is capable to predict the characteristics of both the heat release of combustion as well as NO_x and Soot emissions by using one constant set of model parameters. To a high extent even the quantity of NO_x and Soot emissions could be approximated

very well. Thereafter the most important mechanisms of combustion and emissions formation were conducted on the basis of the sub-reactions in the zones and it could be concluded that the varieties of zone reactions depict the overall performance and emissions characteristics of the engines.

As a follow-up of applying the multi-zone-combustion-model, this paper is focusing on the effects of basic engine control parameter settings on performance and emissions. Thus, the fundamentals of thermodynamics and chemical reaction kinetics are again analyzed on the basis of the reaction zones and the effects of control parameter settings on performance and emissions are discussed.

In-cylinder Diesel engines exhaust emissions are mainly controlled by turbocharging, charge air cooling, EGR, EGR cooling (all of these defining the thermodynamic state of the cylinder charge at intake valve closing), and fuel injection characteristics (such as injection pressure, timing, and multiple injections). From a basic research point of view these measures can be separated into 3 causal effects: (1) mixture formation, which determines the concentration of reactants in individual zones, (2) charge dilution by inert gas species and (3) the actual sequence of the combustion process which is controlled by the kinetics of various chemical reactions. In the real engine these effects usually overlap, and different effects come to the fore depending on the operating condition.

The computational MZCM investigations presented in this paper analyze different combustion strategies by means of their causal effects. Emphasis is laid on changes of thermodynamic conditions which affect heat release and emission formation. Thus, the characteristics of cycle related data such as thermal efficiency, process temperatures, pressures, and resulting emissions as function of changes in engine settings can be predicted.

SHORT DESCRIPTION OF THE MULTI ZONE MODEL

The multi-zone combustion model (MZCM) that is used in this work has been introduced and discussed in detail in [22]. To provide an extensive collection of the sub-models that are used, but to prevent unnecessary redundancies, the mathematical formulations can be found in the [Appendix](#) of this paper. The present work concentrates on the interrelations of these sub-models in the scope of changes of engine parameters.

It is to be noted that the MZCM only calculates the high pressure part of the engine process from Intake Valve Closing (IVC) to Exhaust Valve Opening (EVO). Therefore the model requires as an input the thermodynamic conditions at start of high pressure cycle and appropriate fuel injection characteristics. The thermodynamic state at IVC takes into account the relevant engine parameters turbocharging, exhaust gas recirculation (EGR), charge air and EGR cooling,

valve timing, etc. and is derived either from measurements or from one-dimensional model codes such as AVL's BOOST.

MODELING OF THE REACTION ZONES IN THE MULTI-ZONE MODEL

The mechanisms of the combustion process in the MZCM are shown for a single zone in [Figure 1](#). A zone is generated at the very time-step a fuel parcel is injected into the combustion chamber. It initially consists of pure liquid fuel. Due to the mechanisms of primary and secondary breakup [5, 7] the liquid core disintegrates into single droplets. After that breakup point the continuous processes of mixture formation and evaporation commence which finally leads to combustion.

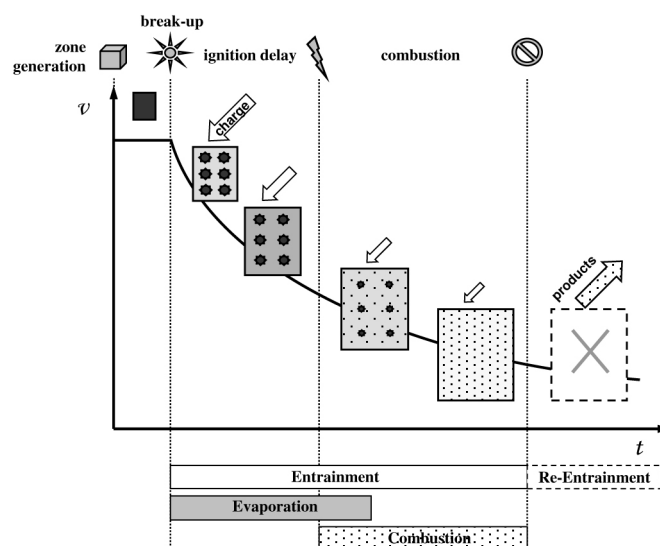


Figure 1. Mechanisms of Mixture Formation and Combustion in the MZCM

The mixing of fuel with the surrounding cylinder charge finds its model-representation in the entrainment of charge into the zones. Simultaneously the liquid droplets heat up from the surrounding hot charge and evaporate. Once a combustible mixture is generated, chemical ignition delay elapses which is calculated separately for each zone. The combustion itself is described by an Arrhenius type kinetic approach.

After completion of combustion the spray zones are summarized to a "Burned-Gas" zone. These combustion products are then recycled together with the fresh charge back into the reaction zones. This mechanism of Re-Entrainment is an important extension to the original Hiroyasu model. A detailed description of the Re-Entrainment mechanism is given in the next chapter.

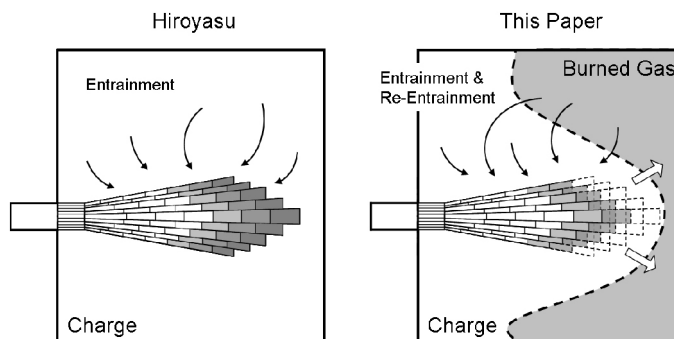


Figure 2. Comparison of Model Conceptions regarding Entrainment and Re-Entrainment

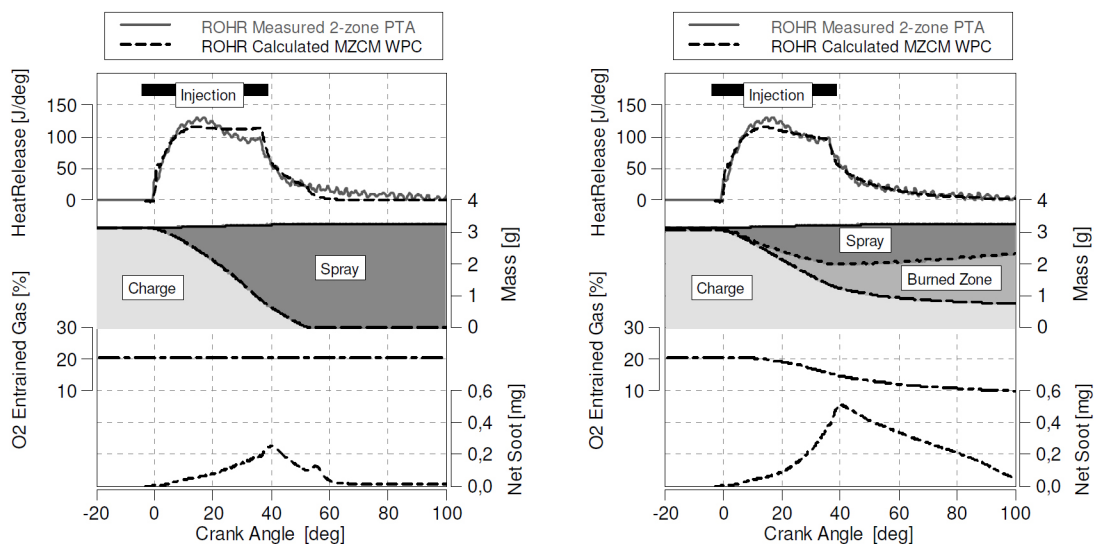


Figure 3. Comparison of calculation results with two different Entrainment mechanisms: (left) Basic Entrainment Model; (right): Extended Model with Re-Entrainment

RE-ENTRAINMENT OF BURNED MASS

The original Hiroyasu approach does not consider heat and mass exchange between the reaction zones. The only actual mass transfer is the unidirectional entrainment of the cylinder charge into the reaction zones (Figure 2). This is a strong simplification which may cause the problem that all oxygen of the cylinder charge is used up and thus stops the process even though there is plenty of oxygen left inside some of the zones. Due to this discrepancy a "Burned-Gas" zone was introduced which absorbs all burned zones but recycles part of them together with the fresh charge back into the reaction zones by the entrainment mechanism. The dosage of burned re-entrainment mass into the fresh charge is controlled by one parameter.

Figure 3 demonstrates the effect of the Re-Entrainment mechanism on the calculation process. It shows a comparison between the two calculation modes in one operating point. In the basic entrainment calculation mode (left) the charge mass is entirely entrained into the spray and therefore consumed at $\sim 52^\circ$ crank angle, which leads to a premature termination of the

combustion. In the Re-Entrainment calculation mode (right) the later injected zones obtain their entrainment mass from both the fresh charge zone and the burned zone. This has two effects: (1) the charge zone is no more entirely consumed, and (2) since combustion products in the burned zone hardly contain oxygen, the mean oxygen concentration of the entrained mass drops (shown in the traces 'O2 Entrained Gas' in Figure 3).

This second effect of suppressed oxygen supply for the later injected zones has special relevance for the calculated soot emissions, as demonstrated by the comparison of the 'Net Soot Mass' traces in Figure 3. In the initial phase of combustion the net soot mass in the cylinder shows a similar progress in both calculation modes. However, by introducing the Re-Entrainment concept soot oxidation is suppressed in the later phase (starting from $\sim 30^\circ$ Crank Angle) due to the lower oxygen supply. This effect is more pronounced at high load points with low global air excess ratio which in general produce more soot. This is the reason why the Re-Entrainment strongly affects the calculation of soot emissions, primarily its characteristics versus engine load.

FUNDAMENTALS OF THERMODYNAMICS AND REACTION KINETICS

The following considerations concentrate on the thermodynamic change of state of the reaction zones in the multi-zone model. The main relevant change of state occurs during combustion when fuel and oxygen react and the temperature increases up to a region that is relevant for emission formation. Of course this process depends on the composition and state of the zones in the moment of ignition which is predefined by the mixture formation processes, i.e. entrainment and evaporation.

EFFECT OF CHARGE DILUTION ON LOCAL COMPOSITION AND ADIABATIC TEMPERATURE OF THE REACTION ZONES

Due to the heterogeneous nature of the (conventional) diesel engine combustion, global values such as the global lambda value or EGR Rate are not directly relevant for the processes that take place locally in different areas of the spray. The local thermodynamic state and composition is rather defined by mixture ratio of fuel and charge and the species concentrations. In the MZCM the heterogeneous concentration field is represented by the distribution of fuel and charge within the different reaction zones of the spray. This is schematically represented in Figure 4. Thus, in terms of composition, the zone is divided into a fuel vapor mass m_{fv} and a zone charge mass m_{ch} . The ratio of fuel mass to charge mass results from the interaction of the mixture formation mechanisms: entrainment and evaporation. The composition of the zone charge mass however is equal to the cylinder charge up to the moment of ignition¹.

To unambiguously define the composition of a zone two values are required: the oxygen concentration of the zone $x_{O_2}^{zone}$ and the zone lambda value λ^{zone} . The zone lambda value results from the ratio of actual oxygen mass to stoichiometric mass.

A first approximation for the temperatures that occur during the process is the Adiabatic Isobaric Flame Temperature (AIFT). It represents the theoretical temperature of a zone at an instantaneous and complete combustion under isobaric conditions.

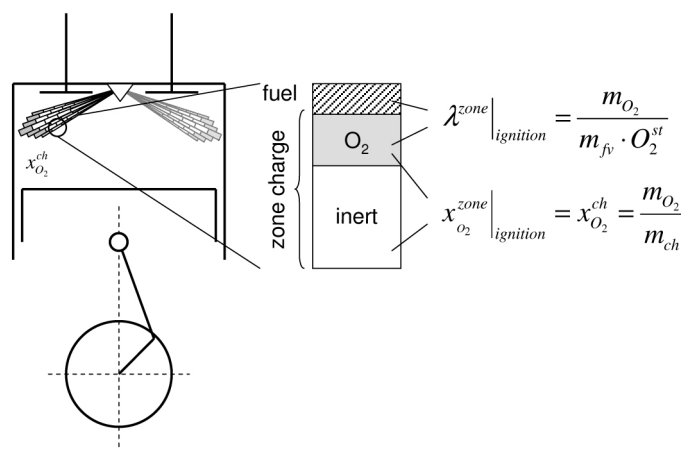


Figure 4. Schematic Representation Definition of Zone Composition and Effect of Charge Dilution

The AIFT is calculated from the fuel energy that is released by the reaction and the mass or heat capacity respectively that needs to be heated up. In the case of $\lambda > 1$ a complete combustion of the fuel is assumed. At higher lambda value the overall mass that needs to be heated up increases which reduces the AIFT. For lambda values < 1 the lack of oxygen limits the amount of fuel that can take part in the reaction. In that case it is assumed that only that part of the fuel reacts which is given by the stoichiometric ratio. Intermediate species of the reaction which occur with incomplete combustion such as CO are not considered. As a part of the fuel remains unburned the released energy is reduced. Therefore the AIFT has its highest value at near stoichiometric conditions which is a result of the highest ratio of induced energy to thermal inertia.

With increasing charge dilution the same amount of oxygen involves a higher fraction of inert species. Hence at the same lambda value the mass of the package increases with decreasing oxygen concentration. These inert species increase the thermal inertia without participating in the reaction.

Figure 5 plots the calculated values for the AIFT as a function of zone lambda for different initial oxygen concentrations. The initial boundary conditions have been chosen to $T_0 = 1000 \text{ K}$, $p = 100 \text{ bar}$ (It is to be noted, that $x_{O_2}^{ch} = 0.233$ corresponds to pure air). In reality the combustion does not occur instantaneously and under isobaric conditions. The influence of the actual process on the zone temperature characteristic is discussed in the following sections.

¹ If the Re-Entrainment mechanism is considered, the composition assembles from the concentrations of the fresh charge zone and the burned zone with respect to the ratio of fresh charge entrainment to burned gas entrainment.

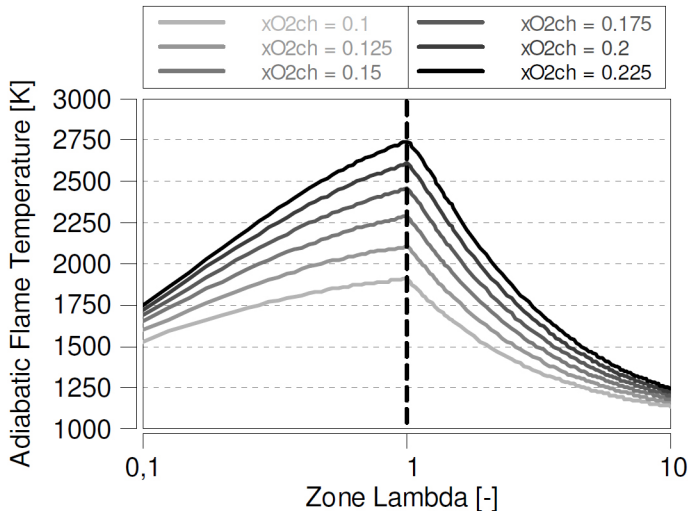


Figure 5. Adiabatic Isobaric Flame Temperature (AIFT) as a Function of Lambda for different Gas Phase Oxygen Concentrations

EFFECT OF THE NON-ISOBARIC COMBUSTION PROCESS ON PEAK TEMPERATURE

It is well accepted that an increase of peak combustion pressure e.g. at an advanced combustion timing leads to higher peak temperatures which enhances NO formation. In this context it is important to note that the AIFT discussed in the previous chapter is nearly independent from the absolute pressure level of the process. This indicates that the simplification of an isobaric combustion that is made for the approximation of the theoretical combustion temperature does not entirely describe the actual process in a reciprocating engine. Here the combustion takes a certain time and consequently the pressure changes due to the heat release and the piston movement. Thus for the peak temperatures not only the absolute pressure level is relevant, but also the course of the process.

To demonstrate the influence of a varying pressure during combustion, an exemplary process is defined. We assume an initial state of 1000K and 100bar and apply (1) an isobaric heating and (2) an isentropic compression to 200bar. These two changes of state are carried out as given and in reverse order.

Figure 6 shows the changes of state in the Temperature-Entropy Diagram. The process plotted in grey starts with the isentropic compression (points 0 → 1) and continues with the isobaric combustion (points 1 → 2). The second process (black line) applies these changes of state in reverse order (0 → 1' → 2'). It can be clearly seen that the second process ends at a higher temperature.

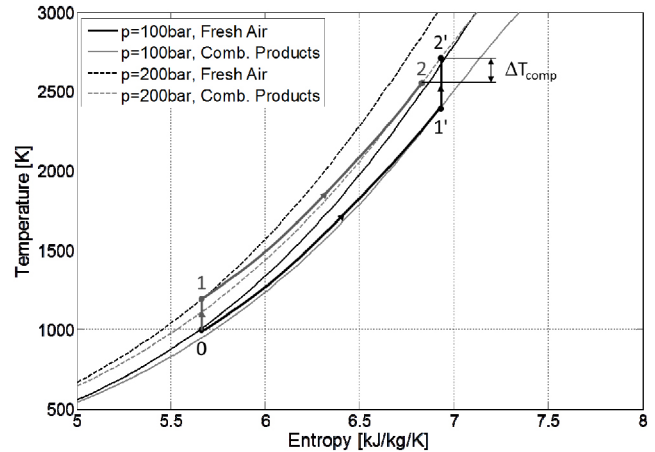


Figure 6. Different Course of the Combustion Process of a Reaction Zone in the T-s Diagram Initial State: $T=1000\text{K}$, $p=100\text{bar}$, $\Lambda=1.25$, $x_{\text{O}_2}=0.2$

From this example it can be concluded that the process cycle influences the peak temperature of combustion in a way that an early heat release with a subsequent compression leads to the highest temperatures. This is an important finding because the combustion is always exposed to the compression and expansion strokes enforced by the piston which thus has a high influence on its characteristics. This is shown in more detail at the description of engine control characteristics below (e.g. timing swings).

EFFECT OF CHARGE COMPOSITION AND ZONE STATE ON COMBUSTION OF A SINGLE PACKAGE

In the MZCM the heat release in the reaction zones is calculated by a reaction kinetic type approach. The equation of Jung [2] is used which is shown in a modified form in eq. (1). Herein the educts concentrations are expressed in terms of mass fractions of fuel vapor and oxygen. The reaction term ' k ' is an equation of the Arrhenius type which additionally considers the density (expressed by p/T_i) as pre-exponential term.

$$\frac{dx_{fb}}{dt} = \frac{d}{dt} \left(\frac{m_{fb}}{m_i} \right) = \underbrace{K_b \cdot \frac{p}{T_i}}_{\text{Reaction Term 'k'}} \cdot e^{\frac{-1200}{T_i}} \cdot \underbrace{x_{fv} \cdot x_{o_2}^{1.5}}_{\text{Educt Concentrations}} \quad (1)$$

The reaction term ' k ' can be reformulated and expressed in logarithmic form with $K_b' = \ln(K_b)$, eq. (2). Due to the consideration of the density in the pre-exponential term, the rate is a function of temperature and also pressure.

$$\ln(k) = \frac{-1200}{T_i} + \ln\left(\frac{p}{T_i}\right) + K_b' \quad (2)$$

The combustion reaction determines the history of temperature and species concentrations in the individual zones which are relevant for the formation of NO_x and Soot. The following considerations concentrate on the impact of the chemical reaction on the evolution of zone temperature and species concentration during the combustion process. Therefore we assume a closed system with given initial state and species concentrations. This demonstration example considers one imaginary zone at start of combustion and assumes that the entire fuel is available as vapor and that there is no heat and mass transfer to / from the surrounding charge zone. The composition of the combustion zone is defined by its fuel-air excess ratio (lambda) and by the oxygen concentration which initially corresponds to that of the cylinder charge, as represented above in Figure 4. During combustion the pressure is assumed to be constant.

Under these conditions the interrelations of stoichiometry and reaction kinetics determine the evolution of temperature and species concentrations. The progression of species conversion during combustion is characterized by the mass fraction of fuel burned ' x_b ', which is defined as

$$x_b = m_{\text{fuel}}^{\text{burned}} / m_{\text{fuel}}^{\text{total}}$$

Figure 7 shows the characteristics of combustion in an Arrhenius-type plot for the given initial conditions: $T=1000\text{K}$, $p=100\text{bar}$ (remaining constant), $x_{\text{O}_2\text{ch}} = 0.2$ for different lambda values. The dashed lines represent the reaction rate characteristics versus temperature at given zone concentrations defined by x_b . Surprisingly the reaction rate at constant x_b decreases with increasing temperature. This is caused by the density in the pre-exponential term which for constant pressure is reciprocal to the temperature, see eq. (1) above. (For a constant density the reaction rate increases with increasing temperature and the characteristics would show straight lines in the Arrhenius plot.)

In the actual combustion process, temperature and oxygen concentration change during the reaction. With increasing x_b the temperature increases according to the released energy. One would assume that due to the higher temperature the combustion rate gets faster. However at the same time fuel vapor and oxygen are consumed. This is mathematically represented in a weakening of the educts concentration term in eq. (1) above. In Figure 7 the full lines show the combustion characteristics under consideration of the interrelation of temperature and reactant concentrations during the reaction. It can be seen that the highest reaction rate occurs at start of combustion (i.e. at $x_b = 0$ to 0.1) due to the high concentrations of all educts. Towards the end of combustion the reaction rate drops significantly (logarithmic scaling!) as at least one of the reactant concentrations approaches zero asymptotically.

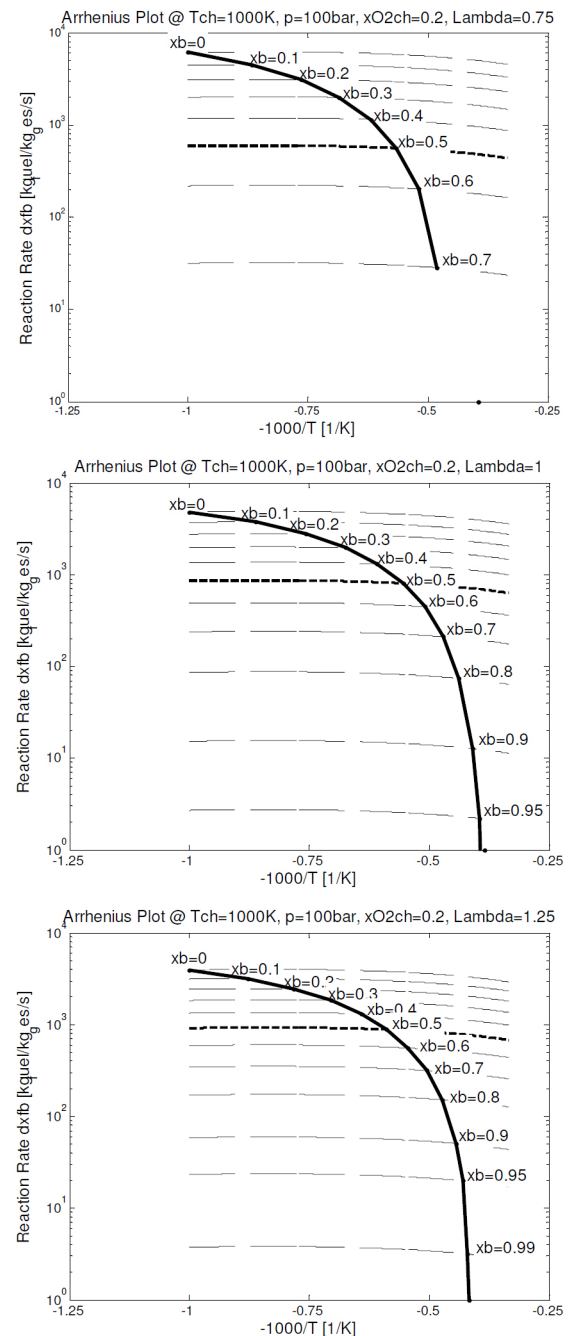


Figure 7. Theoretical Evolution of Combustion Rate of a Spray Package during Combustion in Arrhenius-Type Plot Comparison of $\lambda=0.75$ vs. $\lambda=1$ vs. $\lambda=1.25$

The zone lambda value defines the concentrations of fuel vapor and oxygen in the zone, so it has the most significant influence in the reaction rate and its evolution. Figure 7 compares the characteristics of combustion reaction for three zones with different lambda values. The initial reaction rates are in a similar order of magnitude. However it can be observed that the reaction rate drops faster at small lambda values. This becomes visual focusing on the lines of 50% fuel

burned ($x_b = 0.5$) which are highlighted. In the case of $\lambda < 1$ x_b can only reach values up to the λ value = 1, so part of the fuel remains unburned. The case of $\lambda = 1.25$ has the highest reaction rates throughout the combustion. At $x_b = 0.95$ to 0.99 the reaction rates are significantly higher than e.g. in the case of $\lambda = 1$. This fact is especially relevant in the late burnout phase.

However, the combustion of a single package is fast compared to the global heat release rate. So the characteristics from Figure 7 cannot be transferred to the global heat release rate in the cylinder. The global heat release rate results from the sum of heat release in all zones and is highly determined by the transport processes of the reactants to the zones as discussed in [22].

EFFECT OF THERMODYNAMIC BOUNDARY CONDITIONS ON NO FORMATION

The main relevant inputs to the Zeldovich mechanisms are temperature and equilibrium concentrations of the participating species. Figure 8 shows the molar fractions of O and O_2 calculated from chemical equilibrium as a function of zone λ for different initial zone oxygen concentrations. For the calculations the temperature equals the AIFT shown in Figure 5. The availability of O_2 increases dramatically when λ becomes > 1 which results from the combustion stoichiometry. Atomic oxygen predominantly occurs when first there is plenty of oxygen available and second when additionally temperatures are high enough for dissociation. This is the case in the area right above stoichiometric conditions.

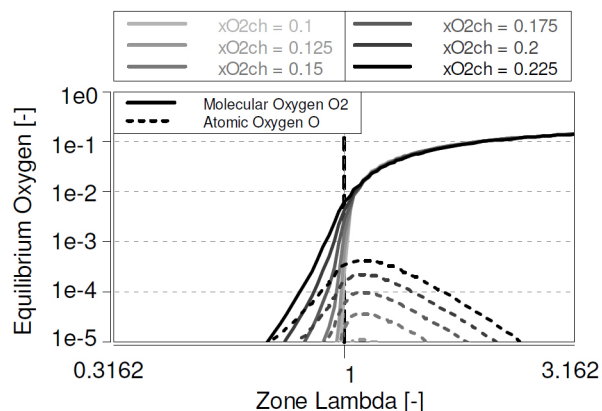


Figure 8. Equilibrium Concentrations of O and O_2 as a Function of λ for different Initial Zone Charge Oxygen Concentrations at corresponding AIFT

Figure 9 shows instantaneous NO formation rates calculated with the extended Zeldovich mechanism. The boundary conditions temperature, pressure and composition are the same as for the results above. The maximum NO formation rate is right above stoichiometric conditions at

$\lambda = 1$ to 1.1 . This results from the combination of high temperatures along with availability of oxygen. The NO formation dramatically drops at lower oxygen concentrations which results from the lower combustion temperature.

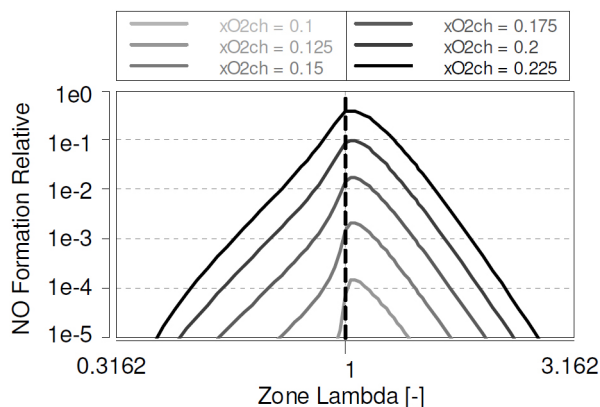


Figure 9. NO Formation acc. Zeldovich ($p=100\text{bar}$, $\alpha=0.5$)

Figure 10 summarizes the previous results. It shows the NO formation rate as a function of adiabatic flame temperature. In the plot oxygen concentration (full lines) and λ values (dashed lines) are represented as iso-lines.

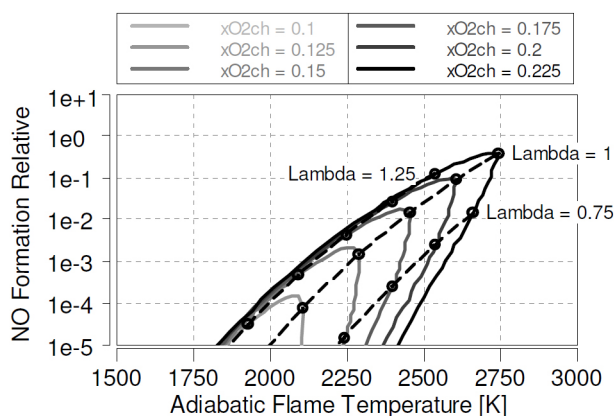


Figure 10. Theoretical NO Formation Rate Zeldovich Mechanism as a Function of Temperature for different λ and Oxygen Concentrations

It is a characteristic of diffusion combustion that part of the heat release is limited by the mixing process of oxygen and fuel. So, it has to be assumed that in most cases there are areas within the spray that burn at stoichiometric conditions and therefore cause the highest rate of NO formation. The only practical way to reduce stoichiometric combustion temperatures is to limit combustion temperatures by means of charge dilution causing the reduction of the oxygen content xO_{2ch} .

- ... Field of all Spray Zones in the Temperature / Lambda Diagram at the given phi-angle
- ... Zones which refer to the Spray Package 'a=3' injected at -9 degCA (see picture on the right)

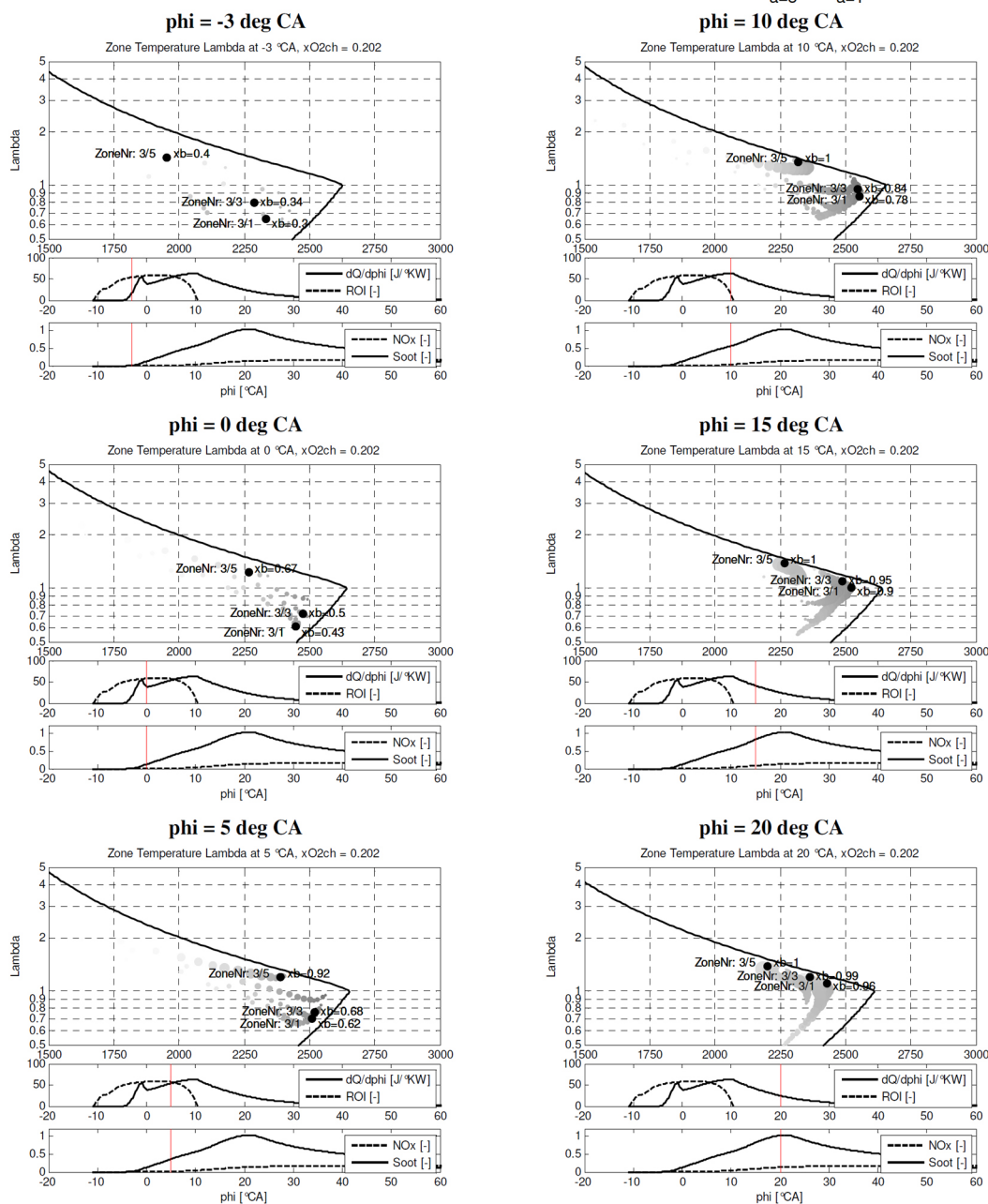
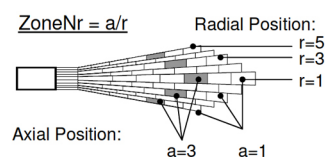


Figure 11. Temporal Evolution of the Spray in the Temperature and Lambda Field - Comparison of 3 Zones (highlighted) injected at the same Time at different radial positions in the spray

TEMPORAL DEVELOPMENT OF SPRAY DURING COMBUSTION

To demonstrate the evolution of the spray combustion in the MZCM the evolution of all reaction zones in the field of temperature and lambda have to be observed. This is shown in Figure 11 for one specific case at different crank angle

positions. In these views on top of each diagram again the line of the adiabatic flame temperature is shown as a function of lambda, though in a clockwise rotated view of Figure 5. The underlying state for the calculation of the AIFT is the current charge zone state (temperature, pressure and oxygen concentration). The intermediate plot shows the crank angle position relative to the injection rate and heat release.