

A Zero-Dimensional Phenomenological Model for RCCI Combustion Using Reaction Kinetics

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ABSTRACT

Homogeneous low temperature combustion is believed to be a promising approach to resolve the conflict of goals between high efficiency and low exhaust emissions. Disadvantageously for this kind of combustion, the whole process depends on chemical kinetics and thus is hard to control. Reactivity controlled combustion can help to overcome this difficulty. In the so-called RCCI (reactivity controlled compression ignition) combustion concept a small amount of pilot diesel that is injected directly into the combustion chamber ignites a highly diluted gasoline-air mixture. As the gasoline does not ignite without the diesel, the pilot injection timing and the ratio between diesel and gasoline can be used to control the combustion process.

A phenomenological multi-zone model to predict RCCI combustion has been developed and validated against experimental and 3D-CFD data. The model captures the main physics governing ignition and combustion. The direct diesel injection is modeled using Hiroyasu's packet approach, where all packets are treated as thermodynamic zones. After the end of injection, mixture formation is modeled as a process dominated by turbulent mixing with mass transfer from zone to zone. Therefore, an algebraic turbulence model has been implemented and compared to 3D-CFD turbulence data. As RCCI combustion is kinetically controlled, heat release is solely modeled using reaction kinetics. To account for chemical reactions a reduced mechanism is used and each zone is considered as a constant volume reactor.

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INTRODUCTION

The simultaneous reduction of fuel consumption and pollutant emissions, namely NO_x and soot, is the predominant goal in modern engine development. In this context, homogeneous low temperature combustion concepts, namely HCCI (Homogeneous Charge Compression Ignition) [1, 2] or PCI (Premixed Compression Ignition) for diesel engines and CAI (Controlled Auto Ignition) [3] for gasoline engines are believed to be among the most promising approaches to resolve the conflict of goals between high efficiency and low exhaust emissions.

Disadvantageously, in both CAI and HCCI concepts, the whole combustion process is kinetically controlled. Thus, there is no trigger like an ignition spark, which could be used to control the ignition and thereby the combustion process. In contrast, ignition and the following combustion process strongly depend on the composition of the cylinder charge, as well as its temperature and pressure history. As these three parameters are all linked together and do strongly influence each other,

controlling low temperature combustion is a challenging task. Reactivity controlled combustion can help to overcome the aforementioned difficulties. In the so-called RCCI (reactivity controlled compression ignition) combustion concept a small amount of pilot diesel is injected directly into the combustion chamber and ignites a highly diluted gasoline-air mixture (see Figure 1).

As the diluted gasoline-air mixture does not ignite without the diesel, the ratio between diesel and gasoline as well as the pilot injection timing can be used to control the combustion process [4, 5, 6, 7, 8, 9]. When the diesel is injected early in the compression stroke, temperature and pressure are still low and the diesel does not ignite directly after injection, but mixes with the surrounding lean gasoline-air mixture. The homogenization of the diesel enhances the long ignition delay and combustion phasing is retarded. Due to the strong dilution of the cylinder charge in conjunction with the high homogenization of the diesel temperatures during combustion stay well below 2000 K, thus NO_x and soot emissions are very

low. If injection is carried out too early during the compression stroke the diesel completely homogenizes and no ignition occurs. Late injection timings on the other hand lead to strong diesel stratification, yielding a two stage combustion process which is likely to show severe knock and high NO_x emissions [7]. For RCCI combustion phasing can not only be controlled by the diesel injection timing but also by the ratio of the amounts of diesel and gasoline. Higher fractions of diesel lead to advanced combustion phasing, whereas small amounts of diesel slow down the combustion process [8]. Altogether it can be summarized that RCCI to a great extent relies on the stratification versus homogenization of diesel and therewith the stratification of ignitability. The stratification can be easily controlled by the diesel direct injection. But, developing transient control strategies still remains a challenge. Numerous engine subsystems such as the turbo charger system, the EGR system and the combustion process closely interact with each other and show high inter-dependencies [9]. Altering one of these subsystems to experimentally evaluate a new control strategy or a new engine design concept is time consuming and cost-intensive.

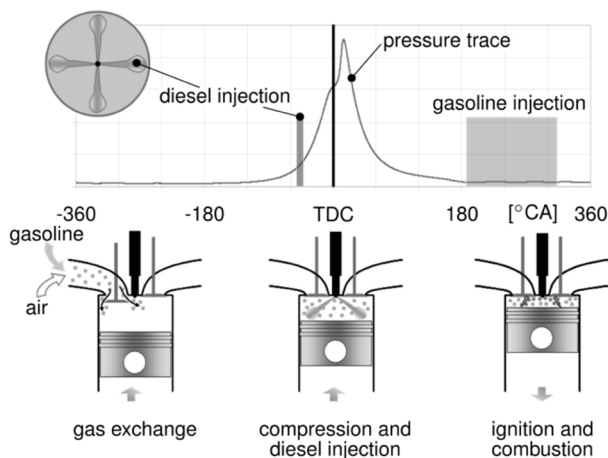


Figure 1. Realization of the reactivity controlled compression ignition (RCCI) combustion concept

Generally, engine cycle simulation can be a valuable tool to ease and speed up the development process of new combustion systems. Numerous models describing diesel [10, 11, 12, 13, 14], premixed flame [15, 16], dual fuel [17, 18, 19, 20] and even kinetically controlled combustion [21, 22, 23, 24] have been developed over the years. But, until now there is no combustion model that is able to predict RCCI combustion, and thus engine cycle simulation cannot substantially contribute to the development of this promising new dual-fuel combustion concept. For this reason a zero dimensional phenomenological combustion model, which is able to predict the RCCI combustion process in terms of its engine power output and heat release rate under different operating conditions, has been developed. Therefore, the relevant processes of mixture formation, ignition and combustion have been simplified in such a manner that they still correctly describe the ongoing physical phenomena, and thus can predict the effects of any change in boundary conditions.

3D-CFD SIMULATIONS

To build a theoretical basis for the present zero-dimensional model, and to further support its development process, 3D-CFD simulations were performed. Altogether, four different load points with different engine speeds and loads were examined thoroughly and compared to experimental data [25]. The experimental investigation was carried out on a four stroke single cylinder engine. The technical engine data is given in Table 1 and the four load points are defined in Table 2.

Table 1. Technical engine data of the single cylinder engine used for model validation.

Stroke x bore	mm x mm	90.4 x 82
Displacement	L	0.477
Connecting rod	mm	145.5
Compression ratio	-	16.7:1
Number of valves	-	4
Inlet valve open	°CA a TDC	-376
Inlet valve close	°CA a TDC	-132
Exhaust valve open	°CA a TDC	112
Exhaust valve close	°CA a TDC	376

Table 2. Load points used for model validation.

		LP1	LP2	LP3	LP4
Indicated mean effective pressure IMEP	bar	3.4	5.3	5.3	5.3
Speed	1/min	1900	2300	1900	1500
Injection strategy	-	Single	Double	Double	Single
Start of diesel injection	°CA a TDC	-46	-66/-46	-57/-37	-42
Injection pressure	bar	500	500	500	500
Gasoline mass fraction	%	70	87	85	90
EGR	%	0	0	0	0

The 3D-CFD simulations were carried out using KIVA-3 [26]. The standard k- ϵ -model was used to predict turbulence. The heat release rate was calculated using the same reduced reaction mechanism [27] that was employed in the 0D-model. The mechanism consists of 41 species and 130 reactions. It is derived from the combination of reduced mechanisms for n-heptane and iso-octane. The mechanism has been validated for different blends of these surrogates and it has been shown that the coexistence of the two fuel components can be modeled successfully.

Experimental work [28] and numerical studies [29] indicate that for RCCI with low equivalence ratios there is no flame propagation thus, no such model was used, either for the 3D or for the 0D simulations. The injection model, which is described in more detail in [30], is based on gas jet theory, and thus allows using a rather coarse grid. The mesh used for the

present CFD simulations is shown in Figure 2. It covers a sector of 51.4° and consists of approximately 10,000 cells at IVC.

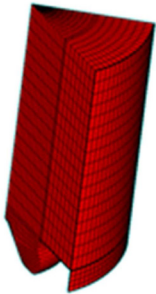


Figure 2. CFD mesh at IVC

As the heat release rate in the KIVA simulations solely relies on reaction kinetics (see above), the initial conditions at IVC are of crucial importance. Therefore, a GT-Power engine system model of the single cylinder engine was developed and validated against experimental data. The pressures, temperatures and compositions at IVC from this model were used as input for the KIVA runs. But, even with detailed system models like GT-Power, some uncertainties in terms of model accuracy remain. When considering simulation results for the whole engine these uncertainties might be negligible, but they can have a considerable impact on the temperature and composition at IVC. In this context, one source of uncertainty within GT-Power is the heat transfer from the hot inlet valves to the fresh charge. It is common practice to account for this extra heat transfer by multiplying the modeled heat transfer from the wall of the inlet port by a constant factor [31]. To estimate the effect of this modeling approach on the conditions at IVC for load point LP 1, different adjustment factors in a range from 0.1 to 5 were explored. The wall temperature was set to the coolant temperature of the test engine. The heat release rate was directly calculated from the experimental pressure data and was later on used in the engine system model. Figure 3 shows the comparison of data from the different 1D simulation runs against corresponding experimental data. Especially regarding the pressure trace, the different simulation runs cannot be distinguished from each other, and the accordance with the experiment is very good. On the other hand temperatures at IVC vary considerably. Despite a variation in temperature of 10 K, the mass flow rate shows only a maximum deviation from the measured value that is less than 5 %. Altogether, all simulation runs would be considered to be in good agreement with the experimental data.

Regarding the calculation of heat release with a reaction kinetics model, it should be noted that a difference in initial temperature of 10 K can completely change the combustion process. In this context, Figure 4 shows the pressure traces and heat release rates from KIVA simulations for LP 1 with different initial temperatures. As can be seen from the figure, an increase of initial temperature of only 7 K results in a large change of combustion phasing and a clearly higher peak

pressure. With even higher temperatures at IVC the combustion phasing is further advanced and the combustion duration reduces remarkably.

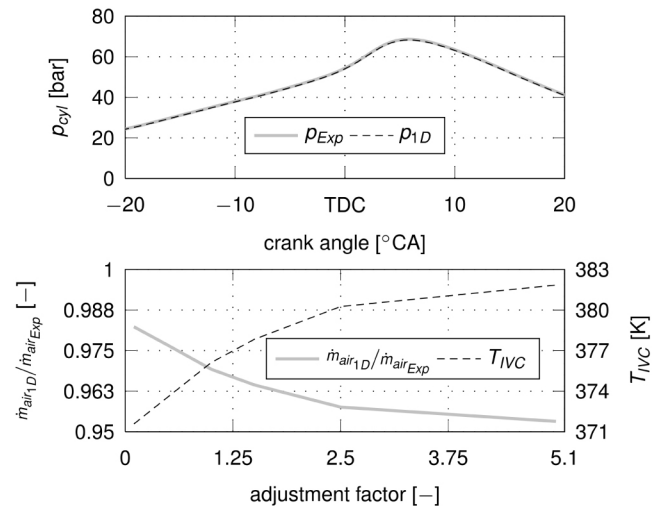


Figure 3. Influence of the wall heat transfer adjustment factor for load point LP 1: Experimental pressure trace, p_{Exp} , against the pressure, p_{1D} , from the corresponding 1D simulations (top), predicted air mass flow rate and temperature at IVC (bottom).

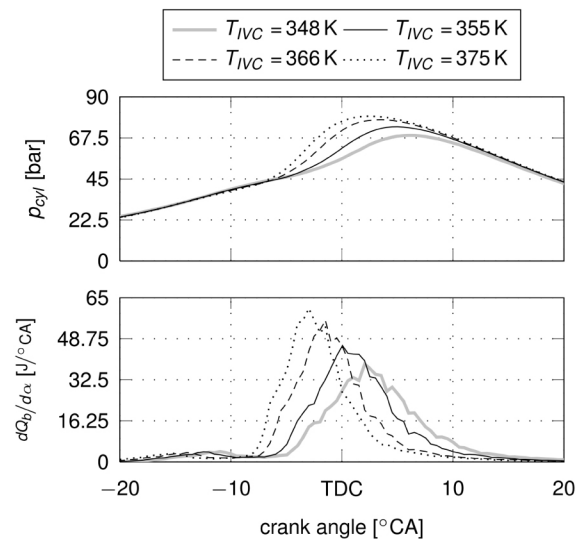


Figure 4. Pressure traces, p_{cyl} , and heat release rates, $dQ_b/d\alpha$, from KIVA simulations with different initial temperatures.

These results show that reaction kinetics are very sensitive to temperature and that even with a detailed 1D engine system model uncertainties regarding initial conditions remain. For this reason the GT-Power model was only used to generate a first estimate for the internal residual gas fraction, which was then used together with the measured pressure, air mass flow rate and gasoline mass to determine the temperature and composition at IVC. By slightly adjusting the residual gas fraction, the conditions at IVC could be adapted in such a way that the CFD results better matched the experimental data.

Figure 5 compares the 3D-CFD pressure traces and heat release rates for the four load points defined in Table 1 with the corresponding experimental data. For all CFD simulations the

residual gas fractions lie in a range between 4.4-9.8 %. Considering the pressure, a good agreement between the experimental data and the CFD simulation results can be seen. Especially in terms of combustion phasing, the heat release rates are also well predicted, even though the maximum values are fairly over predicted. Considering pollutant emissions a satisfying agreement with the measured data could be achieved. As the focus of this work lies on the development of a zero-dimensional combustion model, the correct prediction of pressure and heat release rate has been considered to be sufficient. Thus, no further attempts to improve the prediction of pollutant emissions have been made.

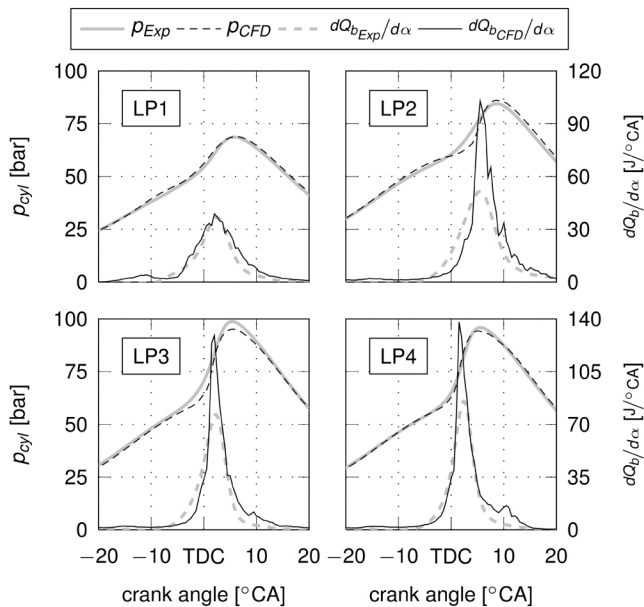


Figure 5. Predicted 3D-CFD pressure traces, p_{CFD} , and heat release rates, $dQ_{b,CFD}/d\alpha$, against corresponding experimental data for the four different load points defined in Table 2.

Due to the injection of diesel directly into the combustion chamber, for RCCI there will be a certain stratification of diesel concentration and therewith a stratification of ignitability. In this context, to further investigate the RCCI-combustion process, the computational cells of the CFD model were subdivided according to their equivalence ratio into 10 groups. For each group the diesel mass fraction, μ_D , the adiabatic mixing temperature, T_{mix} and the lower heating value, LHV were determined. Figures 6 and 7 show the evolution over time of T_{mix} and LHV as a function of equivalence ratio.

As the cylinder content is initialized as being completely homogeneous, the only way different equivalence ratios can develop is because of the direct injection of diesel. Thus, there is a clear correlation between diesel mass fraction and equivalence ratio. Cells with lower equivalence ratio contain less diesel than cells with higher equivalence ratio. Taking this into account, regarding temperature, it is clear that after the end of injection and before the start of combustion cells with higher equivalence ratio show slightly lower temperatures (see Figure 6). These cells have a higher diesel concentration and, as the injected diesel has a much lower temperature than the

surrounding cylinder gas, the mixing of the diesel with the cell content leads to a temperature drop. But, the more dominant effect is from the diesel evaporation. The heat of evaporation is taken from the cell, which further reduces its temperature. Interestingly, cells with lower temperatures, but higher diesel concentration or higher equivalence ratio, start to react first which can be seen by the earlier rise of temperature for these cells. This trend can also be observed from the course of the lower heating value LHV in Figure 7. Before chemical reactions start to considerably consume diesel, cells with higher equivalence ratio, or more diesel, show higher heating values. As soon as combustion starts the heating value in cells with higher diesel concentration decreases rapidly. In this context the reduction of the LHV is a measure for the advance of the chemical reaction. Furthermore, it can be seen that for this rather low load point the very lean cells of the gasoline zone hardly react at all.

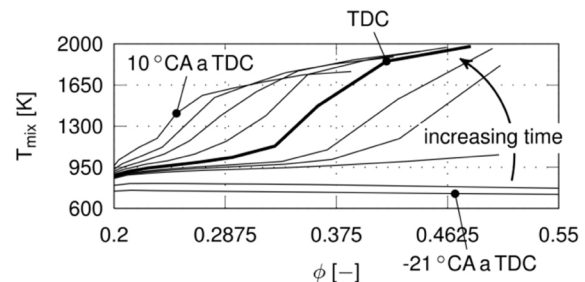


Figure 6. Evolution over time of adiabatic mixing temperature, T_{mix} , in the CFD cells as a function of equivalence ratio, ϕ .

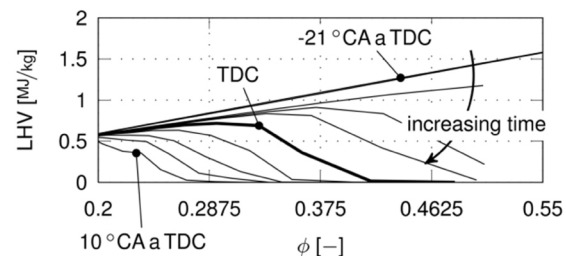


Figure 7. Evolution over time of the lower heating value, LHV, in the CFD cells as a function of equivalence ratio, ϕ .

For the load points LP 2 to LP 4 a very similar behavior could be observed. Thus, it can be summarized that the injection of diesel leads to stratification of equivalence ratio, temperature and ignitability. Despite their lower temperatures, chemical reactions start first in cells with higher diesel concentration. This complies with the results from [29] where through the use of optical measurement techniques and numerical methods it was shown that for RCCI, stratification of diesel is much more influential than temperature stratification. In addition, in [7] the measurement of OH-luminescence and Mie-scattering endorsed the statement that combustion starts in regions with higher diesel concentration. Taking all this into account, together with the fact that for the CFD simulations the cylinder charge was initialized as being completely homogenous and still could satisfyingly predict the combustion process, it can be argued that temperature stratification is not the dominating effect for RCCI combustion. Therefore, it might be neglected.

without adding too much inaccuracy to the zero-dimensional RCCI combustion model. On the other hand modeling mixture formation or diesel stratification seems to be crucial.

MODEL DEVELOPMENT

Formulation

As outlined above the dual-fuel RCCI combustion concept to a great extent relies on the in-cylinder stratification of ignitability induced by diesel direct injection. Hence, the modeling approach for mixture formation results in multiple zones that reflect this stratification. Heat release is then predicted using reaction kinetics for arbitrary mixtures of diesel and gasoline, modeled respectively, as n-heptane and iso-octane. Even though temperature stratification might be present, it is not considered in the model.

Before diesel is injected the cylinder content comprises only a homogeneous gasoline mixture. Thus, only one zone, the so-called gasoline zone, is considered. As soon as diesel is injected multiple zones are created. The diesel injection is modeled using the packet approach first proposed by Hiroyasu [32, 33]. Each packet is treated as an individual thermodynamic zone that entrains the surrounding lean gasoline mixture. Due to this mixing process and due to evaporation each packet consists of gasoline, diesel, air and, if applicable, recirculated exhaust gas (EGR). The entrainment into the spray is not evenly distributed among all packets, yielding lower entrainment rates for zones closer to the spray axis. This, in turn, leads to stratification of diesel with richer packets in the spray core and leaner packets on the edge, surrounded by the lean gasoline zone. After the end of injection the entrainment rate into the packets is modeled considering the in-cylinder turbulence intensity. To calculate ignition and subsequent heat release all zones are treated as perfectly stirred constant volume reactors. Reaction kinetics are modeled using a reduced mechanism for arbitrary mixtures of n-heptane and iso-octane [27]. Cantera [34] version 1.8 served as the chemical kinetics solver. Figure 8 summarizes the model schematically.

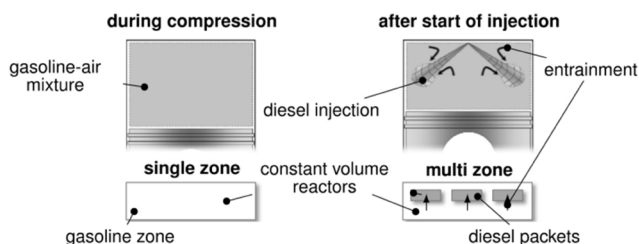


Figure 8. Schematic conception of the RCCI combustion model.

Mathematical Formulation

As outlined above the newly developed combustion model considers a system of multiple chemically reacting zones. The solution of the resulting stiff differential equation system is carried out in a two-step procedure. At the beginning of each

time step the current state of each zone (pressure, p , temperature, T , and a vector, X , holding the mole fractions of each species) is passed to Cantera, which then solves the reaction mechanism and returns the new state of the zones. With these new states the so-called engine system solver accounts for the compression, heat fluxes due to wall heat transfer, mass fluxes over the system boundaries (i.e., diesel injection) and mixing of the zones. Further change of composition due to chemical reactions is not considered. Altogether, this decoupling procedure can be seen as if the chemical reactions and the subsequent macroscopic change of the system are not related to each other. Figure 9 summarizes the coupling between the engine system solver and Cantera.

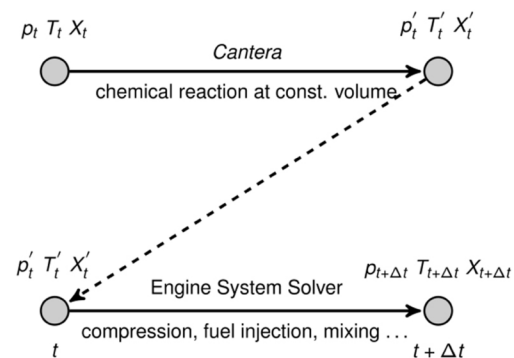


Figure 9. Coupling between the reaction kinetics solver Cantera and the thermodynamic engine system solver.

Engine System Solver

In reciprocating combustion engines time, t , and crank angle, α , are linked through the rotational speed, n . Thus, both quantities are equivalent. As most models or physical processes depend on time rather than on crank angle, the derivative with respect to time should be favored. For the sake of simplicity in the following equations the total derivative with respect to time d/dt or crank angle $d/d\alpha$ is given in its short form d .

Pressure trace analyses, as well as working process simulations are based on the first law of thermodynamics and the equation of state. In this work the gas equation for ideal gases is used. The thermodynamic system is defined by the walls of the combustion chamber and can be divided into an arbitrary number of sub-systems, the so-called zones. Mass can be transferred in any direction between zones, whereas inter-zonal heat fluxes are not allowed. If pressure is assumed to be equal in all zones, and if furthermore only gaseous species are considered, a simple system of ordinary differential equations can be derived for each zone:

$$p dV_z + m_z \frac{\partial u_z}{\partial T_z} dT_z = \sum_j dQ_{zj} + \sum_j (dm_j^* h_j^*) - \sum_j (dm_j^* u_j)$$