Premature Flame Initiation In SI Engines: Modeling Studies On The Role Of Residual Gas

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1 Introduction

Downsizing, i.e., generating more mechanical power per displacement, is an important concept for reducing fuel consumption and emissions of piston engines [1]. It is mostly achieved by turbo-charging and/or by high compression ratios, thus increasing the overall pressure and temperature level of engine operation. In recent years, a prominent combustion anomaly has been observed which seems to be characteristic for downsized gasoline engines, namely an uncontrolled, spontaneous initiation of combustion and spread of a flame in early phases of the engine stroke [2]. This phenomenon, often simply termed "pre-ignition", can cause excessively high cylinder pressures with considerable damage potential, and thus poses a severe obstacle for further engine development. These pre-ignition events are, under the conditions which typically exist in the operation of current engines, quite rare. Moreover, their occurrence seems to be completely random; no evidence has been found yet that would allow to predict in a particular engine cycle whether this cycle will pre-ignite or not.

The exact reasons for the onset of this pre-ignition have not been identified yet. Optical observations suggest a localized, point-like initiation of combustion [2], with subsequent deflagrative flame propagation (rather than combustion initiation in an extended, voluminous region as, e.g. typical for knocking engines); this indicates that a local auto-ignition is a key process in premature flame development.

Several phenomena have been discussed as potential sources for localized auto-ignition [2,6] including oil droplets, hot components, and deposits on cylinder walls or piston crowns. Currently, to our knowledge, no single reason explaining the auto-ignition at such an early stage of the engine cycle has been identified yet. It is possible that a combination of different effects causes the pre-ignition.

Understanding the phenomena is hindered by the complex interaction of several processes and physical quantities possibly involved in pre-ignition. In an experiment, it is difficult to precisely control the influencing factors and to vary them independently. This strongly complicates the interpretation of experimental observations, especially in view of the fact that processes like auto-ignition and flame propagation depend in a strongly nonlinear manner on the engine conditions. In view of these difficulties, numerical simulations can be an aid for

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understanding the phenomena. They allow the study of the influence of single parameters on auto-ignition and, in addition, the system behavior can be studied in a wide parameter space. Thus, by modeling studies it is possible to cover most of the expected conditions in the mixture. Complementing experimental evidence with the results of the simulation yields a higher level of interpretability.
In this work, detailed numerical studies on the impact of residual gas (defined here generally as gas that remains in the cylinder between consecutive engine cycles due to scavenging losses) on the ignition characteristics of a fuel-air-mixture under SI-engine relevant conditions are performed.

2 Methodology

The numerical simulations were carried out applying a homogeneous reactor model taking into account detailed chemical kinetics based on the detailed "Primary Reference Fuel"-mechanism by Curran et al. [3,4]. Iso-octane is used as a high-octane number gasoline fuel surrogate. The simulation of engine cycles is performed by computing a transient volume profile defined by the engine geometry and the engine speed. Heat losses to the walls as well as mass losses due to blow-by are not considered in this work, which aims at identifying the key processes of pre-ignition and not to deliver a detailed engine model.
Table 1 displays the chemical composition of the residual gas, which was used in the simulations. It corresponds to the composition of burned gas after the expansion stroke at a pressure of 2.25 bar and 875 K for a stoichiometric initial fuel-air-mixture.

Carbon dioxide, CO_2	19.2 %
Water, H_2O	8.8 %
Nitrogen N_2	71.9 %
Carbon monoxide, CO	$5.0 \cdot 10^{-3}$ %
Oxygen, O_2	$3.25 \cdot 10^{-2}$%
Hydrogen, H_2	$2.2 \cdot 10^{-4}$ %
Hydoperoxide, H_2O_2	$1.54 \cdot 10^{-6}$ %
Hydroperoxy radical, HO_2	$1.34 \cdot 10^{-5}$ %

Table 1: Computed composition of the residual gas at a pressure of 2.25 bar and a temperature of 875 K.

The simulations apply a homogeneous reactor model to describe the mixture in the cylinder. This model can be applied to the whole cylinder, but also to partial volume elements of the mixture. In a real engine, there will generally be incomplete mixing between residual gas and the fuel/air mixture. To account for this effect, the mixture state is represented here by a probability density function (PDF) of the residual gas mass fraction (RGMF). This description is appropriate if the transport processes between regions of differing mixture state are negligible. This applies in the limit of small scalar gradients. Further studies including the influence of transport processes on pre-ignition are subject of current work.
To ascertain how the variance of RGMF can affect the probability of local auto-ignition before TDC (possibly leading to premature flame development), the following procedure is taken: The statistical, spatially varying distribution of RGMF in a cylinder charge is modeled by a β-pdf [7]. In this approach, the mean and the variance of the RGMF distribution are adjustable parameters. Assuming that the mean value of RGMF is 1%, which represents the typically low overall residual gas fraction of turbo-charged engines, the variance of the

RGMF can still be varied. Some distributions with a mean value of 0.01 and various variances are plotted in Figure 1. Very small variances correspond to a cylinder charge with homogeneous RGMF distribution (rightmost curve in Figure 1), very large variances correspond to the unmixed case, i.e., pockets of pure RG embedded into fuel/air mixture (leftmost column in Figure 1).

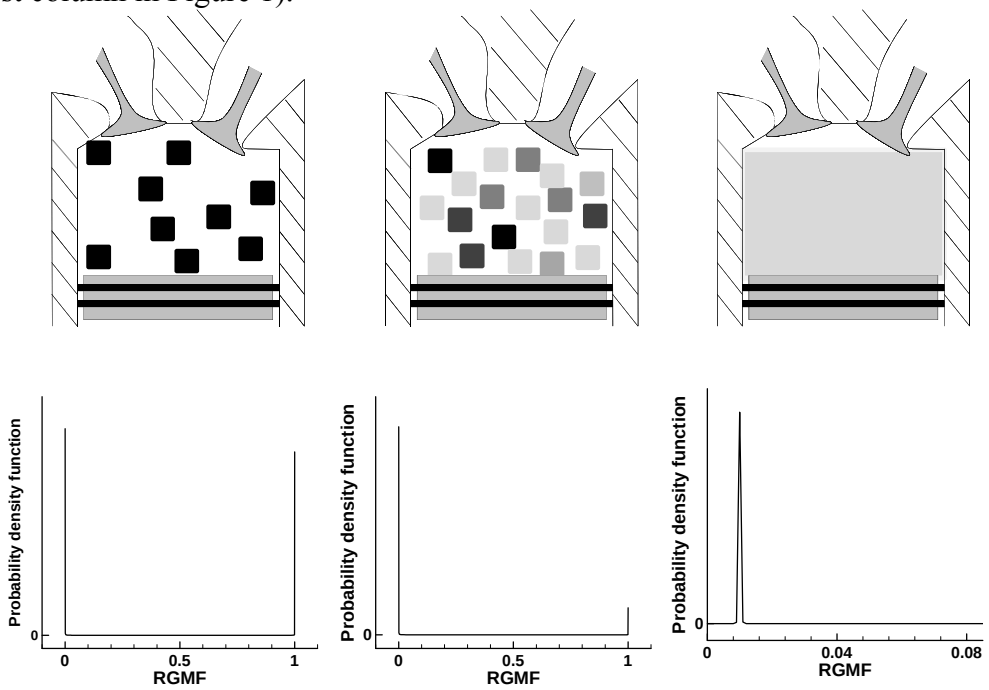

Figure 1: β-PDFs of RGMF with mean 0.01 and various variances (left to right: 0.0098, 0.003, 1×10^{-9}), along with sketches roughly representing the corresponding RG / fresh gas distributions in the cylinder charge. White color represents pure fuel/air mixture, black color represents pure RG and grey areas depict mixed states.

In reality, there will usually be an intermediate case between these extremes, RG being partially mixed with fresh gas (center column in Figure 1). The probability of the event that, in a statistically distributed cylinder charge, a local auto-ignition occurs before TDC (0°CA) can be computed as the integral of the PDF between the limits within which auto-ignition of homogeneous reactors occurs before TDC. This probability depends on the variance of the PDF and also on the residual gas temperature.

3 Results

The assumed engine geometry data is shown in Table 2.

Compression ratio:	10.5
Displacement (single cylinder) / m^3:	$4.96\cdot10^{-4}$
Bore / m:	$8.25\cdot10^{-2}$
Stroke / m:	$9.29\cdot10^{-2}$
Piston rod / m:	$1.45\cdot10^{-1}$
Engine speed / rpm:	1750

Table 2: Engine geometry data

The engine geometry parameters were taken from a production engine (Audi TFSI four cylinders, displacement $1.984 \cdot 10^{-3}$ m^3) that is known to show occasional pre-ignition events in laboratory studies.

The simulations were performed for a set of initial conditions displayed in Table 3. For constant initial pressure, temperature and air-fuel-ratio a variation of the residual gas temperature and ratio was carried out. Figure 2 shows the computed dependence of the residual gas ratio on the crank angle at which an auto-ignition was observed in homogeneous reactor engine simulations. The crank angle corresponding to the onset of ignition is determined by the peak value of the OH-profile. The initial fresh gas temperature was set to 300 K in all simulations and the curves correspond to different residual gas temperatures (see Table 3).

Fuel:	2,2,4-trimethyl-pentane
Fuel-air-ratio λ:	1.0
Intake pressure p0 / bar:	2.25
Intake temperature T0 / K:	300
Residual gas temperature TRG / K:	500, 750, 875, 1000, 1250
Residual gas ratio:	0%, …, 100%

Table 3: Variation ranges of the initial conditions

In the simulations with an initial residual gas temperature of 500 K no auto-ignition was observed. Mixing with residual gas featuring a temperature of 750 K already provokes a considerable acceleration of auto-ignition relative to the case without residual gas. The residual gas has two competing effects: The residual gas dilutes the reactive fuel/air mixture, which tends to delay auto-ignition. On the other hand, residual gas (if it has a higher temperature than the fuel/air mixture) increases the temperature of the mixture, promoting auto-ignition. Depending on the residual gas temperature and the amount of residual gas in the mixture, one of the two effects will prevail.

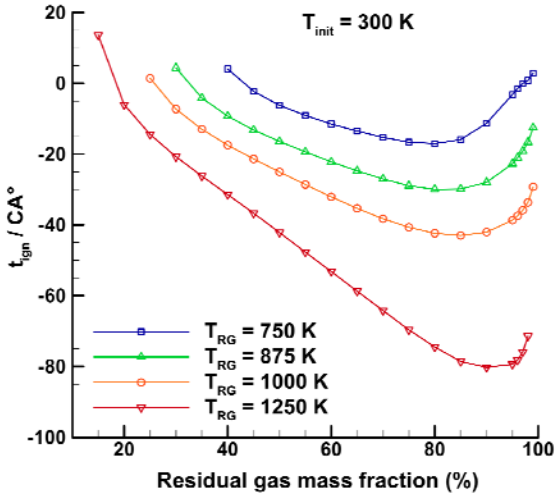

Figure 2: Computed dependence of the residual gas mass fraction (RGMF) on the crank angle at which auto-ignition occurred in homogeneous reactor engine simulations. The curves correspond to different initial residual gas temperatures, as indicated in the legend. 0° CA correspond to TDC.

The above discussed statistical approach is now applied to estimate the pre-ignition probabilities within a certain interval of RGMF. The integration interval was determined by two characteristic residual gas mass fractions. The lower boundary corresponds to the mixture featuring the lowermost RGMF showing an auto-ignition before 0° CA. The second boundary is given by the mixture with the highest RGMF exhibiting a temperature increase of at least 300 K during ignition. Considering the curve representing the mixtures with residual gas of 875 K those boundaries are 45% and 85% respectively. The sensitivity of the pre-ignition probability with respect to the integration limits only becomes significant for very low and very high residual gas mass fractions respectively.
Figure 3 shows the result for the different RG temperatures and various variances. It is seen that the probability of local auto-ignition is zero when the variance is either very low or very high, but can approach higher values at intermediate variances.

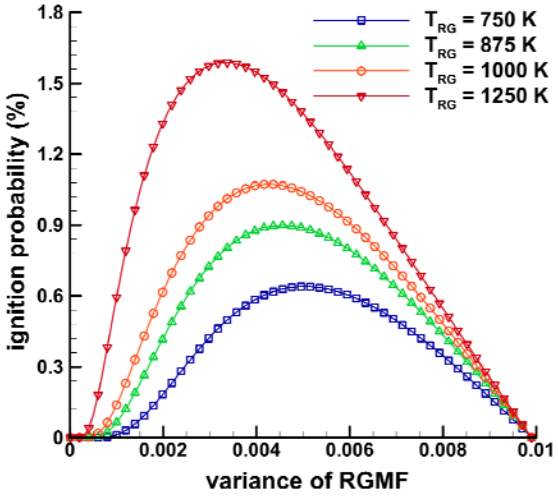

Figure 3: Probability of local auto-ignition in a cylinder charge with statistically distributed RGMF of mean 0.01, as a function of RGMF variance**.**

Overall, the ignition probabilities are quite small (below 1%, unless T_{RG} is excessively high). This is in accord with the experimental observation that pre-ignition [2], at least under typical engine operation conditions, is a very rare event. In case of a very small variance in RG mass fraction, the residual gas is mixed homogeneously with the fresh gas (Figure 3), and hardly any effect of RG on auto-ignition is expected due to the overall small RG content. The probability of auto-ignition is then practically zero. For extremely high RGMF variances, there is no mixing between RG and fresh gas. The cylinder charge then consists of pockets of pure burned gas (which cannot ignite) and pure fresh gas (which, under the conditions studied here, cannot auto-ignite due to its comparably low temperature). In intermediate cases mixed regions representing potential sources of auto-ignition before TDC can exist. Therefore, the probability for auto-ignition exceeds zero.

4 Conclusion

Numerical studies were performed applying a homogeneous reactor model to study the role of residual, hot residual gas in the cylinder charge as a possible initiator of pre-ignition in gasoline engines. A simple statistical approach on homogeneous reactors ensembles was taken to estimate the pre-ignition probability in mixtures with inhomogeneous spatial distribution of hot residual gas and negligible influence of transport processes.

If the residual gas in amounts which are typically present in turbo-charged engines (< 1% RGMF) mixes homogeneously with the fresh gas, no considerable effect on auto-ignition and flame development is observed. In contrast, if the residual gas is only poorly mixed with fresh gas, so that locally concentrated, small regions with increased RG content remain in the combustion chamber, the result is a dramatic alteration of the local ignition properties in the mixture. If characteristic values for modern, supercharged gasoline engines of the residual gas temperature and mean residual gas mass fraction are used in the simulations, it is observed that local auto-ignition can occur in an engine cycle well before top dead center, thus possibly initiating pre-ignition. Estimations of the probability of such an event, based on β-PDFs of RGMF, show small probabilities in the order of 10^{-3} that an auto-ignition occurs before TDC, which is in accord with the observed rare and stochastic occurrence of pre-ignition in engines. Based on these results, we conclude that statistical local fluctuations of residual gas mass fractions have to be considered as possible candidates for explaining (and, possibly mitigating) pre-ignition in engines.

Further studies on pre-ignition with inhomogeneous distributions of residual gas in the cylinder charge including the effect of transport processes are subject of current work.

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