Time Dependent Based Mixing Time Modelling for Diesel Engine Combustion Simulations

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1 Introduction

An application of a probability density function (PDF) based stochastic reactor model (SRM) is one of the possible methods to simulate combustion and emissions formation in internal combustion engines (ICE). In the PDF based SRMs the effects of chemical reactions on fluid composition is treated exactly whereas turbulent mixing of the in-cylinder content is modelled. The common feature of existing mixing models, such as IEM or Curl's [1] is that the turbulent time scale – mixing time, must be given. The mixing time that is seen as an inverse of the mixing intensity is a crucial parameter of the mixing model. The history of the mixing time influences the level of inhomogeneities in in-cylinder mixture composition and temperature. This in turn directly affects SRM's capabilities in predicting engine-out emissions and performances.

In turbulent processes occurring in ICE the mixing time is not constant. In some applications, such as in studies of homogeneous charge compression ignition (HCCI) combustion, the SRM performs accurately enough when the mixing time is approximated by the constant value over the entire engine cycle (e.g. [2]). In the case of Diesel engines however, our preliminary studies (e.g. [3]) indicate that an improvement of the SRM's performance can be achieved if time dependency to the description of the mixing time is considered.

In this work a model describing the mixing time as a function of time during the engine cycle is applied. The model by means of a combination of linear and exponential functions defines regimes of various mixing intensity respectively to the physical and chemical processes occurring during the cycle. This mixing time history has been incorporated into the Curl's mixing model and used in the stochastic reactor model for direct injected engines (SRM-DI) to simulate performances of Diesel engines.

2 Modelling and Simulation Approach

2.1 Numerical Model – The SRM-DI

The SRM-DI is a part of chemical kinetics based modelling environment DARS [4]. It is a zero-dimensional model of physical and chemical processes relevant to the simulation of engine in-cylinder

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processes. The model considers gas inside the cylinder as an ensemble of particles. Each particle has a chemical composition, temperature and equiweighted mass, that is, each particle represents a point in a composition space for species mass fraction and temperature. Particles can mix with each other and exchange heat with the cylinder walls. Scalars, species mass fraction and temperature, are considered as random variables and are described with probability, using PDF. The turbulent mixing process is modelled using Curl's mixing model with mixing time being time dependent. The content of the cylinder is subjected to pressure and volume changes, chemical reactions, heat transfer, and mixing.

2.2 Time Based Mixing Model Setup

To account for different mixing time during engine cycle, the cycle was divided into a few regimes. The regimes were defined on the basis of the heat release results (Figure 1) characteristic for Diesel combustion. The heat release rate data was used because it in a quantitative way describes the combustion process and allows for distinguishing its different phases. To gain further insight into the combustion process, the heat release results were supported by the available from literature ([5]) 3D CFD based calculations of scalar dissipation rate relevant to Diesel engine combustion (Figure 2). In simulation of turbulent reactive flows the scalar dissipation rate describes the influence of the flow field on chemistry. It has the dimension of an inverse time and therefore represents the inverse of a diffusion time scale [6]. The decay of the scalar dissipation rate indicates thus how the mixing process develops, i.e. it represents mixing intensity. By analogy, in the SRM based simulations, the diffusion time (called further mixing time) can be taken to close the setup of the mixing model. Successful 3D CFD calculations (e.g. [7]) have been performed using single representative interactive flamelet, based on a single, volume average scalar dissipation rate. This suggest that the single scalar dissipation rate can be used as an indicator on how to construct only one function that describes mixing intensity over entire engine cycle.

Based on the heat release data four different regimes of the Diesel combustion and engine cycle can be distinguished (Figure 1). These are I – a compression phase and eventually expansion, until the start of fuel injection, II – fuel injection phase that includes also the premixed combustion, III – a regime corresponding to mixing controlled combustion, and IV – a regime relevant to late combustion phase and later expansion until exhaust valve opening. The most important are regimes II and III where, among others, the combustion process is initiated, the spray develops, the majority of energy is released and emissions are formed.

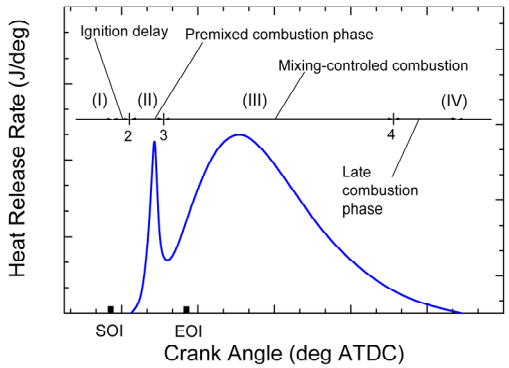

Figure 1. Exemplary heat release rate diagram with different Diesel combustion phases as given in [10].

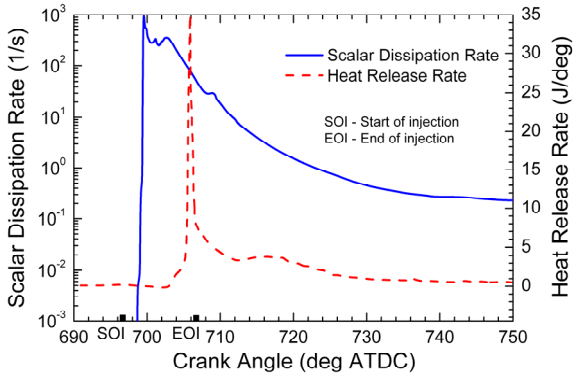

Figure 2. Scalar dissipation rate and heat release results relevant to Diesel combustion (Based on [5]).

An occurrence of the characteristic peak on the heat release diagram in regime II indicates time during engine cycle where the premixed combustion takes place. In this regime the mixing process is expected to be the shortest during the cycle. This regime corresponds to the highest value of the scalar dissipation rate (Figure 2). Initially, within the fuel injection phase, the scalar dissipation rate, (until a

visible heat release rate occurrence) does not change significantly. Therefore, it has been assumed to approximate the mixing time during the fuel injection period by constant value linear function.

The diffusive combustion mode – regime III in Figure 1, is the longest phase of the Diesel combustion. It corresponds to a regime where a decay of the scalar dissipation rate is observed (Figure 2). In this work the decay of the scalar dissipation rate, i.e. also the profile of the mixing time is assumed to follow an exponential function. This is one of possible methods to describe a decay of a passive scalar in turbulent flows (e.g. [8]). From the scalar dissipation rate data, it is assumed that the exponential character of the mixing time starts where injection ends and ends approximately where the mixing controlled combustion phase is finished.

It has been assumed that in regimes I and IV mixing intensity can be represented by constant value linear functions. This simplification is due to the fact that in these regimes, the most important processes, i.e. combustion and emissions formation have not started yet or have already finished. The value of the mixing time for the fourth regime is taken as being the same as value that is found at the end of the third regime. The same value is assumed for the first regime.

Following the above description, the mixing time during the complete engine cycle can be described as a sum of four mixing sub-processes (Figure 3) relevant to different physical and chemical processes during engine cycle as defined in Figure 1.

$$\tau_{IVC-EVO}(t) \propto A_0\big|_{\tau_I} + t'\big|_{\tau_{II}} + \left(A_0 - A_0 \exp\left(-B \cdot t\right)\right)\Big|_{\tau_{III}} + A_0\big|_{\tau_{IV}} . \quad (1)$$

In this equation t is a time during the cycle that is translated into crank angle. The A_0 is an unknown parameter. It affects the value of the mixing time in regime I and, together with parameter B in regimes III and IV. The parameter B is given as $B=ln(2)/t''$, where t'' denotes the half time for the exponential part of the mixing time. The parameter t' defines intensity of the mixing during the fuel injection phase. The parameters A_0 and B are the most influential on model's performance. In general, the A_0 influences the anchorage of the exponential part of the mixing time whereas B affects its slope.

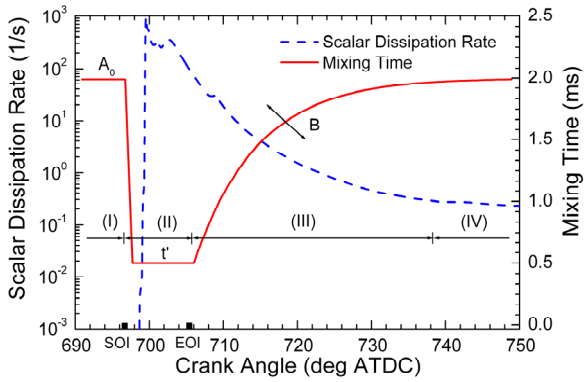

Figure 3. Concept of the mixing time changes during the cycle plotted against scalar dissipation rate from Fig. 2.

It should be noted that duration of each of the mixing sub-process (τ_I, τ_{II}, τ_{III}, τ_{IV}) are also model parameters that can be subjected to some fine adjustments from their defined above values. In general however, the mixing time for the complete engine cycle can be described (Eq. 1.) using two parameters, i.e. A_0 and t''. Other model parameters, including the duration of each of the mixing sub-process and also parameter t' can be well assigned prior to simulations. This, in turn means that in practice, the complete SRM-DI based engine model can be validated against experimental data using only these two parameters A_0 and t''.

3 Simulation Results – Model Validation

3.1 Engine Data and Test Case Definition

Simulation results refer to the experimental data from a direct injection Volkswagen engine. Engine specifications are listed in Table 1. In Table 2 the operating condition is defined. The engine was operated at low speed and part load condition with IVC (Inlet Valve Closure) at 144 CAD BTDC (Before Top Dead Center) and EVO (Exhaust Valve Opening) at 130 CAD ATDC (After Top Dead

Center). The engine was fuelled with n-heptane that was injected (17.2 mg) as a single-shot injection using the common rail system. Measured emissions, relevant to the operating condition given in Table 2, included NO, NO_2, HC, CO and CO_2.

Table 1 Engine basic specification

Engine Type	DI Research Engine
Bore (mm)	81
Stroke (mm)	95.5
Displaced volume (cm^3)	492
Compression ratio (–)	16.3:1
Fuel	n-heptane

Table 2 Engine operating condition

Parameter	Value
Engine speed (min^{-1})	2000
Indicated mean effective pressure (bar)	6.9
Start\End of injection (deg ATDC)	-2.0\3.0
EGR (–)	0.33
Lambda (–)	1.8

3.2 Chemical Sub-Model

The chemical kinetics modelling within the SRM-DI engine model is based on the reaction mechanism for n-heptane developed by T. Zeuch et al. [9]. It is a version thoroughly tested and using a variety of data obtained through various experimental techniques. A skeleton mechanism is used. It contains 121 species and 973 reactions, including backwards reactions.

3.3 Engine Model Results

Simulations were performed over the closed part of the cycle. The content of the cylinder was discretized into 200 particles. Default settings in Woschni model were used. The stochastic heat transfer parameter that governs the distribution of the heat transferred over particles was set to 15. The global simulation time step in the operator splitting scheme was set to 1.0 CAD. The vaporisation process in the model is described based on the fuel injection rate, i.e. mixing controlled vaporisation is assumed. To ensure correct timing for the vaporisation rate the input injection rate profile was shifted from the original value –2 CAD ATDC to 1.5 CAD ATDC. The mixing time was set up following the description presented in Sec. 2.2. Engine performance results were taken as average values from computed 100 consecutive cycles.

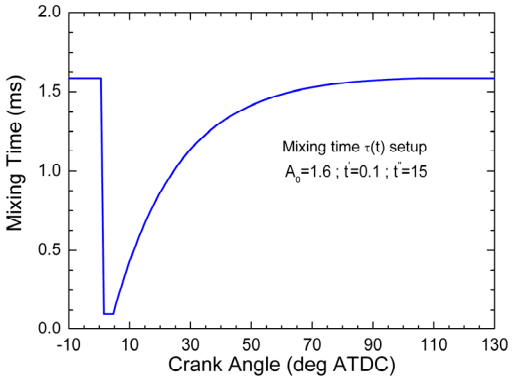

Figure 4. Mixing time model setup relevant to simulation of engine condition from Table 2.

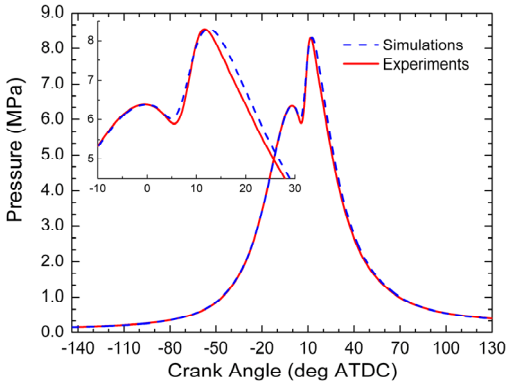

Figure 5. In-cylinder pressure history. Experimental results compared to model results.

In Figure 4 the dependency of the mixing time on time (CAD) during the cycle is presented. The setup of the model was obtained iteratively by adjusting model parameters (following Eq. 1) until the measured results (pressure, emissions, etc.) were matched. In Figures 5 to 9 validation results are presented. The model is capable of predicting in-cylinder pressure (p) and temperature (T) with high accuracy (Figure 5 and 6).

There is a good agreement between simulated and measured maximum peaks of p and T. Also the location, on crank angle basis, of maximum values of p and T is also well captured. These results are well reflected in the heat release rate results (Figure 7.) that provide a deeper insight into the combustion phenomena.

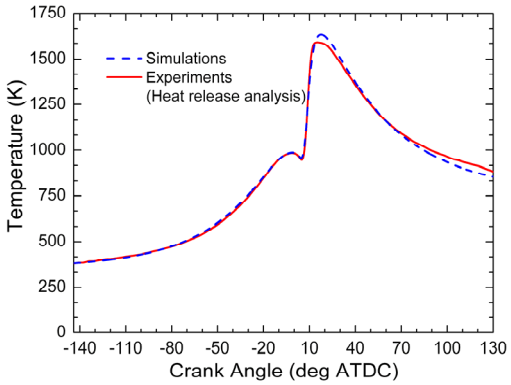

Figure 6. In-cylinder temperature history. Model results vs. data from the heat release analysis on the measured in-cylinder pressure data.

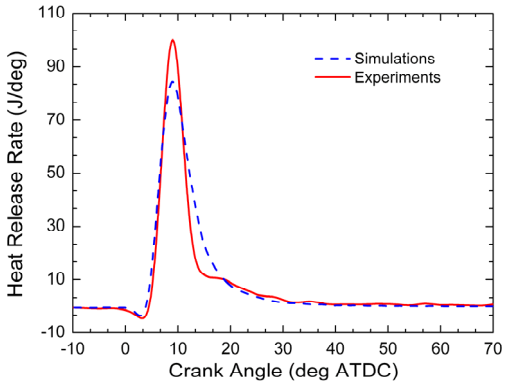

Figure 7. Net heat release rates results from the thermodynamic analysis performed on measured and simulated in-cylinder pressure data

The advantage of the PDF approach in simulating engine performance is revealed in the simulating emissions formation. It is possible to follow the dynamics of the formation process of different species under engine conditions (Figure 8.).

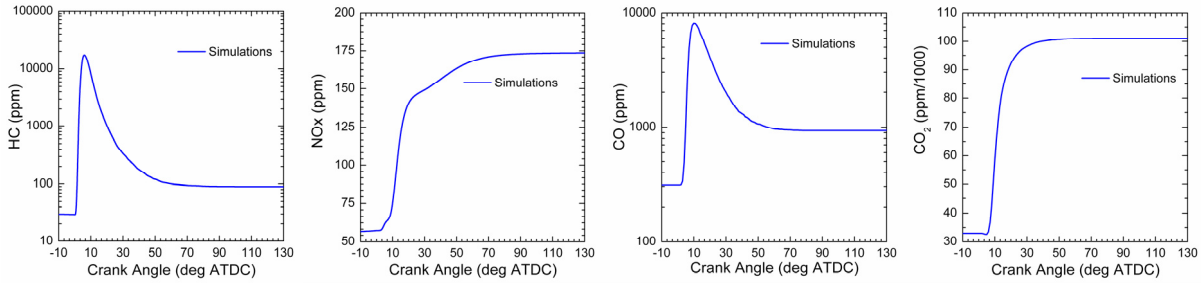

Figure 8. Simulated formation of HC, NO_x, CO, and CO_2 as a function of crank angle.

This can be especially useful for more detailed applications of the model such as, for example investigating ignition delay or start of combustion under engine conditions. The analysis of occurrence of these processes can be supported by information about formation rates of different radicals. This information in turn is obtained from the time based results from the SRM and suitable reaction mechanism.

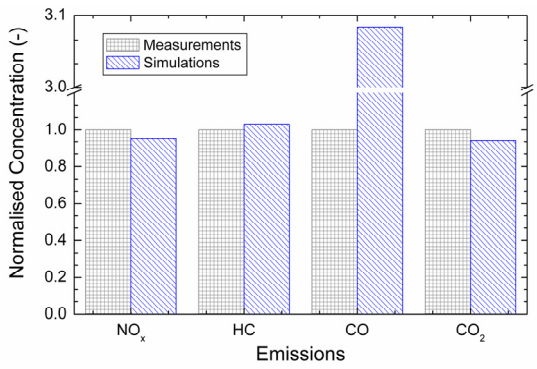

Figure 9. Engine-out emissions. Results for different species at EVO normalized to measured data.

Apart from crank angle based results, the model provides also engine-out emissions in a standard manner, i.e. as cumulative values at EVO. In Figure 9 simulated results for HC, NO_x, CO, and CO_2 are compared with measured data. Introducing time dependency has not only an influence on in-cylinder pressure temperature etc. but it also leads to results of higher accuracy for typical emissions. Especially good agreement has been obtained for total hydrocarbons (HC), NO_x and CO_2.

The relative difference for the considered operating condition does not exceed 5% for HC and NO_x and is 6% for CO_2. Less accurate results have been obtained for CO that is also a source contributing to differences in CO_2. In general however, the results here presented, i.e. engine–out emissions (but also in-cylinder performances), are of high accuracy, especially by the fact that they come from 0-D modelling framework.

4 Summary

The time dependent mixing time model has been proposed and applied as a closure for the Curl's description of the turbulent mixing. The model was incorporated into the Stochastic Reactor Model for Direct Injected engines (SRM-DI) and applied to simulate Diesel engine combustion. The model, being calibrated by means of basically only two, user adjustable parameters, covers completely the closed part of engine working cycle. The effects of the adjustable parameters on model results (pressure, emissions) have been tested. Due to limited length of the extended abstract these results will be included in a full length paper.

By introducing time dependency into the mixing intensity description, the overall capability of the SRM-DI in predicting Diesel engine performance increased. The model simulates in-cylinder parameters such as pressure, temperature, heat release rate, etc. with high accuracy. Especially good results were obtained for engine out-emissions. For NO_x and HC the relative difference between simulated and experimental data does not exceed 5%.

Presented simulation method with time dependency in the mixing process, improves the overall capabilities of the SRM-DI. The method is applicable to various engine related investigations, such as for example, engine performance optimisation or testing fuels performance under Diesel combustion conditions.

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