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Energy Procedia 142 (2017) 4092–4097

Energy Procedia

www.elsevier.com/locate/procedia

9th International Conference on Applied Energy, ICAE2017, 21-24 August 2017, Cardiff, UK

Modelling of soot formation in a diesel engine with the moment projection method

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Abstract

In this work, the recently developed moment projection method (MPM) is coupled with the Stochastic Reactor Model engine code to simulate the formation of soot in a direct injection diesel engine. The simulations take into account convective heat transfer, turbulent mixing, and adopts a detailed chemical mechanism so that the concentrations of soot precursors can be predicted. The soot model considered in this work is based on integration and modification of existing sub-models for soot inception, coagulation, condensation, surface growth and oxidation. The soot moment equations are solved using MPM which has been proven to be accurate and robust. A single-cylinder research version of the Great Wall 4D20 diesel engine with exhaust gas recirculation is modelled for two test cases with different injection timings, injection pressures and fuel consumptions. Simulations are fast (on the order of minutes) and comparison of computed and experimental pressure and heat release rate are in excellent agreement. The amount of soot produced is in qualitative agreement with measurements of diesel smoke opacity.

Peer-review under responsibility of the scientific committee of the 9th International Conference on Applied Energy.

Keywords: moment projection method, stochastic reactor model, diesel engine, soot

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1876-6102
Peer-review under responsibility of the scientific committee of the 9th International Conference on Applied Energy.
10.1016/j.egypro.2017.12.330

1. Introduction

Compared with gasoline engines, diesel engines have the advantages of higher power and lower fuel consumption. However, the formation of soot and other particulate matter (PM) challenges the viability of diesel engines as more stringent emissions standards have been imposed [1]. In order to improve our understanding of the soot formation and destruction mechanisms and to meet the demand for cleaner combustion strategies, modelling and simulation of soot formation in diesel engines are of increasing importance.

The formation of soot is a rather sophisticated physical and chemical process involving gas-phase chemistry, heterogeneous reactions on the particle surface and particle dynamics depending on a wide range of parameters. The literature on soot modelling in engines has been largely restricted to heavily simplified, empirical soot models which are usually incorporated into the Computational Fluid Dynamics (CFD) code KIVA [2]. The majority of these empirical soot models belong to the two-step model of Hiroyasu and Kadota and its variants [3,4]. These soot models have advantages of ease of implementation and low computational costs, however they suffer from a narrow range of applicability and so far have only achieved limited success in capturing soot properties.

At the other extreme, highly detailed soot models have been adopted for the simulation of soot formation. In [5] the soot model is accounted for using SWEEP, a Monte Carlo based population balance solver which is able to accommodate up to thousands of internal coordinates. These not only include bulk soot properties such as soot mass, number density but also the morphology and chemical composition of soot aggregate. However, the extensive use of detailed soot models is inhibited by the high computational cost involved.

Models based on the method of moments are a compromise between the simplified empirical soot models and the very detailed ones in terms of computational efficiency. During the last two decades, numerous moment methods have been proposed, however most of them cannot handle the oxidation process where the smallest soot particles decompose into gas species and are removed from the particle system. Information about the smallest particles is therefore required which is not resolved in most methods of moments. Recently a moment projection method (MPM) has been proposed which directly solves the moment transport equation and has the ability to track the number of the smallest particles [6]. MPM has the advantages of being numerically simple and easy to implement. It has also shown excellent performance in accounting for particle shrinkage which arises due to processes such as oxidation, evaporation or dissolution.

The aim of this work is to present an engine model which can be used to simulate soot formation in a diesel engine. The model is based on the Stochastic Reactor Model (SRM) which includes detailed chemical kinetics, and possesses sub-models for turbulent mixing and convective heat loss [5]. It is able to qualitatively predict the emissions of CO, CO_2, NOx and unburnt hydrocarbons with little computational cost per engine cycle on a conventional desktop PC.

The soot model incorporated into the code is based on the work of Balthasar et al. [7] where the soot particles are assumed to be spherical and five particle processes are considered: inception, coagulation, condensation, surface growth and oxidation. MPM is used to solve the moment transport equations.

The coupled code is used to simulate the combustion process of a single-cylinder GW4D20 diesel engine from Great Wall. Two test cases are applied where engines were operated under different injection timings, injection pressures and fuel consumptions.

The paper is structured as follows. The engine model and soot model are first presented. Then the combined model is used to simulate two diesel engine cases and results are compared with experimental measurements. Finally, some key conclusions are summarised.

2. Model description

2.1. Engine model

The SRM engine code is a spatially zero dimensional model for physical and chemical processes. The model is inspired by the Probability Density Function (PDF) transport methods [5]. It employs detailed chemical kinetics and possesses sub-models for heat transfer, turbulent mixing, piston movement and fuel injection. The SRM has been successfully employed in a number of simulations for internal combustion engines such as a Direct Injection Spark

Ignition (DISI) engine [5] and a port fuel injected Homogeneous Charge Compression Ignition (HCCI) engine [8]. An important concept in the SRM is the so-called 'stochastic particle' which represents a point in phase space for local scalar variables such as species concentrations, temperature and pressure. The engine cylinder charge can be split into an ensemble of stochastic particles to represent the distribution of these variables.

For the simulation of combustion in diesel engines, a very important concern is the in-cylinder mixing intensity which has a significant influence on the mixture inhomogeneity. Selection of a proper turbulent mixing model is especially important when the soot model is described by a quadrature based moment method such as the MPM used in this work. Inappropriate mixing of moments may violate the realisability of the moment set, leading to unphysical results. In this work turbulent mixing is described by a Curl's model in which a pair of stochastic particles is chosen at a time according to a certain probability law characteristic of the particular model and mixed to produce two new stochastic particles [9]. The properties of the two post-mixed stochastic particles are the mean of the properties of the original ones. The Curl's mixing model has been proven to be able to maintain the consistency between the mass density functions based on moments and those based on the particle size distribution.

The SRM model employs a detailed kinetic model for Primary Reference Fuels (PRFs). The chemical mechanism describing the kinetics contains 208 species and 1002 reactions. The formation of soot precursors including pyrene is included.

2.2. Soot model

In this work soot is modelled as a population of spherical particles described in terms of their size, where a particle of size i refers to a particle that contains i carbon atoms. The density of soot is assumed to be a constant of 1800 kg/m^3. The basic physical and chemical processes assumed to be important for the formation of soot are: inception, coagulation, condensation, surface growth and oxidation by OH and O_2. Inception is modelled as the creation of the first soot particle due to the collision of two gas-phase polycyclic aromatic hydrocarbon (PAH) molecules with the rate given as

$$R = kc_i c_j, \tag{1}$$

where k is a pseudo second-order rate constant describing the rate of inception due to the collision of two gas-phase species with concentrations of c_i and c_j. The identity of the PAH species is a model parameter and in this work it is specified as pyrene. The surface processes can be described by the equation

$$W = k_s(s_{i-j}N_{i-j} - s_i N_i), \tag{2}$$

where k_s is a pseudo first-order rate constant describing the rate of a surface reaction that contributes j carbon atoms to a particle, and s_i is the surface area of a particle of size i. The surface growth process is modelled to occur through a repeating cycle of H-radical abstraction and acetylene addition (HACA) mechanism and condensation is the deposition of pyrene onto the soot surface [10]. Oxidation refers to the removal of carbon atoms from the soot particles through surface reactions with molecular oxygen and hydroxyl radical. Coagulation is modelled as the creation of spherical particles due to the coalescent collision of soot particles described by the equation

$$G = \frac{1}{2}\sum_{j=1}^{i-1}\beta_{j,i-j}N_j N_{i-j} - \sum_{j=1}^{\infty}\beta_{i,j}N_i N_{j,} \tag{3}$$

where β is the collision kernel which is dependent on the Knudsen number. In this work soot collision is assumed to occur under transition regime, the coagulation term used is similar to [11].

The main step involved in integrating the soot model into the SRM code consists of associating the soot moment equations with each of the SRM stochastic particles and solving them at each computational time step. Another key ingredient is to link the gas-phase chemistry to the soot particle processes by identifying one or more species in the

chemical mechanism as inception and soot surface reaction species. Detailed information on the coupling between SRM and MPM will be presented in a future paper.

3. Results and discussion

In this section the coupled SRM-MPM codes is used to simulate combustion in a single-cylinder diesel engine from Great Wall (GW4D20). The engine was operating at 1600 rpm with an EGR total mass fraction of 0.2. The engine specification is given in Table 1.

Table 1. Engine specifications.

Bore (mm)	83.1
Stroke (mm)	92.03
Compression ratio	16.7
Displacement (cm^3)	500
Connecting rod length (mm)	145.8

The engine was running under two test cases. The operating conditions are given in Table 2.

Table 2. Engine operating conditions.

Case	SOI (ATDC)	Injection duration (us)	Fuel consumption (kg/h)
1	-9	500	0.67
2	-11	495	0.69

Simulations were run with a time step of 0.2 CAD and 100 stochastic particles. The computation time for the case 1 and 2 was only 546 and 650 s, respectively. In Fig. 1, the predicted in-cylinder pressures and heat release rates are compared to measurements. The overall predictions of both cases are satisfactory.

In Fig. 2, the moment rates of M_0 and M_1 for all processes involving the soot particles for case 1 and case 2 are shown as a function of crank angle. It can be seen that the moment rates for all particle processes shows a sharp increase soon after injection at around 0 CAD ATDC. There is quite a bit of noise because during the combustion process there are great fluctuations in turbulent mixing and rapid reactions of gaseous species. As the combustion process weakens, the moment rate curves become smooth and the rates show a steady decrease. The inception rate in case 1 is larger than in case 2 which leads to the formation of more soot particles. However this gap is eliminated due to a higher oxidation rate observed in case 1. The oxidation rates via O_2 and OH are found to be of the same order of magnitude. The rates show a steady decrease after 0 CAD ATDC as the in-cylinder temperature is decreasing and the oxidation species are being consumed. The moment rates due to other processes (coagulation, condensation and growth) are similar for both cases.

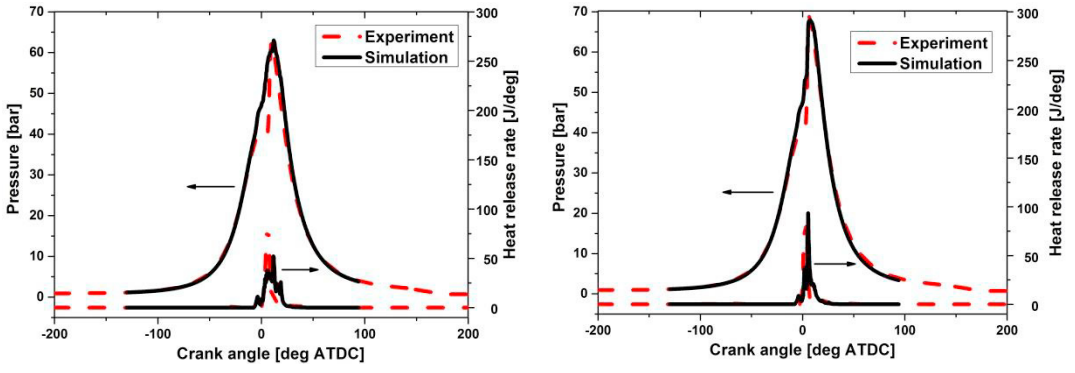

Figure 1. Comparison of predicted and measured in-cylinder pressures and heat release rates for case 1 (left panel) and case 2 (right panel).

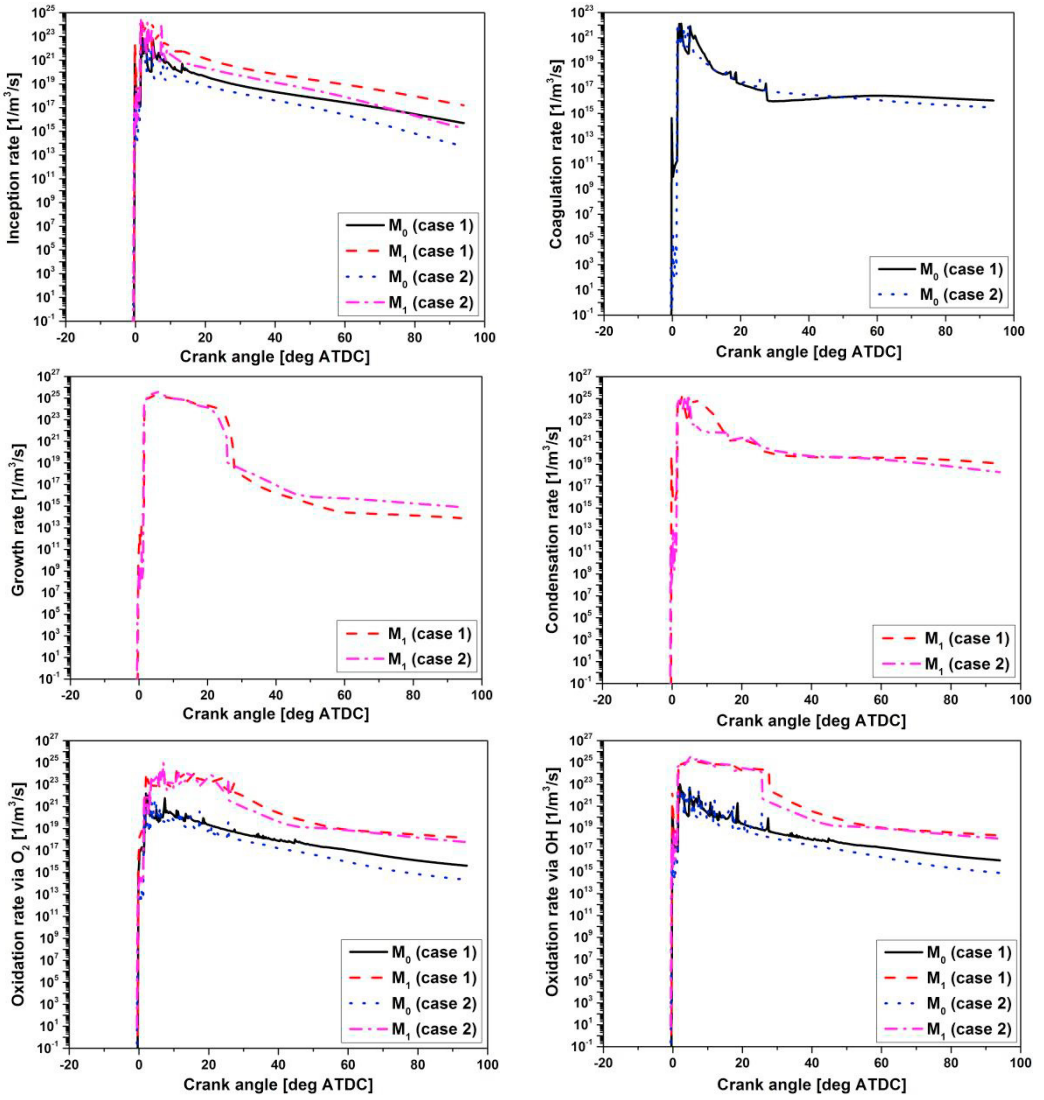

Figure 2. Moment rates of the soot processes considered in the model as a function of crank angle for diesel engine case 1 and case 2.

Figure 3 shows the predicted total soot number and mass for both cases as a function of crank angle. Both cases show similar trends of soot formation. After ignition at around 0 CAD ATDC, a quick build-up of soot is observed due to inception. Then oxidation starts to gain strength and results in a decrease in soot formation. At around 28 CAD ATDC, the soot formation process reaches some sort of equilibrium where the soot number and mass remain constant. Two observations can be made: (1) the final engine-out soot mass for both cases is similar (although that of case 2 is slightly higher) and (2) the concentrations of soot is very low. This is consistent with experimental measurements of diesel smoke opacity which was found to be 0.018 and 0.02 1/m for cases 1 and 2 respectively. It can be concluded that the coupled SRM-MPM code has the ability to predict the trend of soot formation in diesel engines.

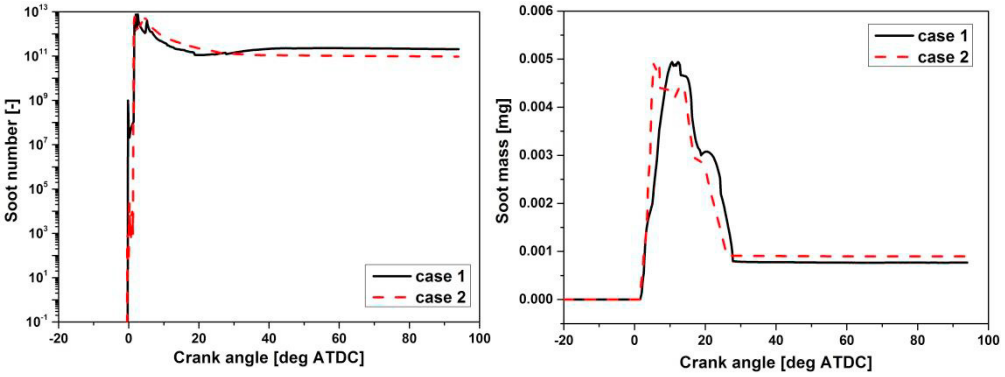

Figure 3. Comparison of predicted soot number and mass between case 1 and case 2.

4. Conclusion

A recently developed moment projection method is coupled with a PDF-based SRM engine simulation code to describe the soot particle dynamics including inception, coagulation, condensation, surface growth and oxidation inside a diesel engine. The simulations adopt a detailed chemical mechanism to describe the formation of gas species, including soot precursors. The turbulence mixing is accounted for using a Curl's model which ensures the realisability of the moment set. The moment projection model, being computationally cheap, enables the study of soot particle number and mass under different engine operating conditions.

We used the integrated code to simulate the combustion process of a single-cylinder diesel engine operated under two different conditions. Through the analysis of the contributions of different particle processes to the formation of soot, simulation results suggest a similar trend of soot formation in both cases. A quick build-up of soot is observed after ignition followed by a steady decrease as oxidation starts to dominate. The predicted engine-out soot mass is similar in both cases with case 2 exhibiting slightly more soot, which is qualitatively in agreement with measured diesel smoke opacity.

Acknowledgements

This research is supported by the National Research Foundation, Prime Minister's office, Singapore under its CREATE programme.

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