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Modelling soot formation from wall films in a gasoline direct injection engine using a detailed population balance model

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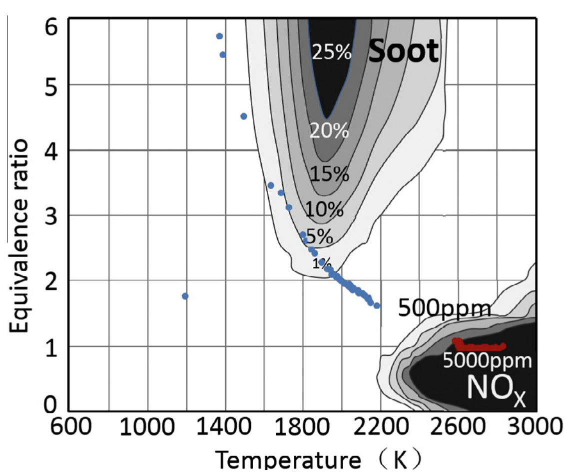
HIGHLIGHTS

- Soot formation from a wall film in a GDI engine is simulated.
- Spray impingement and wall film evaporation models are added to SRM Engine Suite.
- Soot is modelled using a highly detailed population balance model.
- Particle size distributions are measured experimentally.
- Evolution of wall region is shown in equivalence ratio-temperature diagrams.

GRAPHICAL ABSTRACT



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ABSTRACT

In this study, soot formation in a Gasoline Direct Injection (GDI) engine is simulated using a Stochastic Reactor Model (SRM Engine Suite) which contains a detailed population balance soot model capable of describing particle morphology and chemical composition. In order to describe the soot formation originating from the wall film, the SRM Engine Suite is extended to include spray impingement and wall film evaporation models. The cylinder is divided into a wall and a bulk zone to resolve the equivalence ratio and temperature distributions of the mixture near the wall. The combustion chamber wall is assumed to exchange heat directly only with the wall zone. The turbulent mixing within each zone and between the two zones are simulated with different mixing models. The effects of key parameters on the temperature and equivalence ratio in the two zones are investigated. The mixing rate between the wall and bulk zone has a significant effect on the wall zone, whilst the mixing rate in the wall zone only has a negligible impact on the temperature and equivalence ratio below a certain threshold. Experimental data are obtained from a four-cylinder, gasoline-fuelled direct injection spark ignition engine operated stoichiometrically. An injection timing sweep, ranging from 120 CAD BTDC to 330 CAD BTDC, is conducted in order to investigate the effect of spray impingement on soot formation. The earliest injection case (330 CAD BTDC), which produces significantly higher levels of particle emissions than any other case, is simulated by the current model. It is found that the in-cylinder pressure and the heat release rate match well

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Nomenclature

Abbreviations
ATDC After Top Dead Centre
BTDC Before Top Dead Centre
CAD Crank Angle Degree
CFD Computational Fluid Dynamics
CIDI Compression Ignition Direct Injection
DISI Direct Injection Spark Ignition
DMS Differential Mobility Spectrometer
EGR Exhaust Gas Recirculation
GDI Gasoline Direct Injection
HCCI Homogeneous Charge Compression Ignition
KMC Kinetic Monte Carlo
LES Large Eddy Simulation
LIF Laser-Induced Fluorescence
LII Laser-Induced Incandescence
LPDA Linear Process Deferment Algorithm
PAH Polycyclic Aromatic Hydrocarbon
PDF Probability Density Function
PM Particulate Mass
PN Particulate Number
PPCI Partially Premixed Compression Ignition
PRF Primary Reference Fuel
RON Research Octane Number
SI Spark Ignition
SMD Sauter Mean Diameter
SOF Soluble Organic Fraction
SRM Stochastic Reactor Model
TDC Top Dead Centre

Roman symbols
d_0 injector nozzle hole diameter [m]
d_d droplet diameter [m]
D fuel/air binary diffusion coefficient [m^2/s]
$H^{(i)}$ enthalpy in the ith computational particle [J]
La Laplace number [–]
$\dot{m}_{fuel}$ injected mass flow rate [kg/s]
$m^{(i)}_{liq}$ mass of liquid fuel in the ith computational particle [kg]
$M_{tot,w}$ total mass in the wall zone [kg]
$N^{(i)}_d$ number of liquid fuel droplets in the ith computational particle [–]
Δp pressure drop across injector nozzle [bar]
Q_f fuel vaporisation heat [J/kg]
Re Reynolds number [–]
S spray penetration [m]
Sc Schmidt number [–]
Sh Sherwood number [–]
Δt simulation time-step [s]
T temperature [K]
v_{in} normal component of incident droplet velocity [m/s]
$W^{(i)}$ statistical weight of the ith computational particle [kg]
We Weber number [–]
We_c critical Weber number separating spread and splash regimes [–]
$Y^{(i)}_j$ mass fraction of jth species in the ith computational particle [–]

Greek symbols
β ratio of exchange mass flow rate and total mass in wall zone [1/s]
γ droplet rebound/stick split ratio in splash regime [–]
δ thickness of wall film [m]
θ spray cone angle [°]
κ ratio of bulk and wall zone mixing times [–]
ρ_g gas mass density [kg/m^3]
ρ_l liquid fuel mass density [kg/m^3]
μ liquid fuel viscosity [m^2/s]
σ fuel droplet surface tension [N/m]
τ turbulent mixing time [s]
Φ fuel/air equivalence ratio [–]

with the experimental data. The particle size distribution in the simulation has the same order of magnitude as the experimental one. By tracing the particles in an equivalence ratio-temperature diagram, it is demonstrated that the rich mixture near the wall becomes the source of the soot formation as a result of the wall film evaporation.

1. Introduction

Internal combustion engines are of critical importance to transportation and hence global energy demand, and are projected to remain so for years to come [1]. Achieving high energy efficiency and at the same time low levels of pollutant emissions are therefore key drivers of development.

Amongst the various engine types, Gasoline Direct Injection (GDI) engines are becoming the most widely used gasoline engines attributed to their superior efficiency compared with traditional Port Fuel Injection (PFI) engines [2]. Unfortunately, the particle emissions are higher for GDI engines, and it is difficult for the manufacturers to control the particle mass and number below for example the limit value of EURO VI (PM < 5 mg/km and PN $< 6 \times 10^{11}$ particles/km) [3–5]. Additionally, the fine particles, especially the ones with the size less than 2.5 μm (known as PM2.5), have adverse health effects [6]. Thus, it is necessary to determine the source of particles in GDI engines and take measures to reduce the particle emissions.

It is well-known that the engine-out particulate matter from Diesel engines can be divided into two modes by size, the nucleation mode and the accumulation mode [7]. For the nucleation mode, the particles normally have the size ranging between 5 and 50 nm and consist of Soluble Organic Fraction (SOF) and sulphate. Typically the nucleation mode contains 1–20% of the particle mass and more than 90% of the particle number. For the accumulation mode, main part of the particles is dry soot with the size ranging between 100 and 300 nm. It was found by many tests that most of the particles from GDI engines are located in the accumulation mode [8,4,5]. The peak value of the accumulation mode is around 100 nm.

Because of the longer ignition delay and good volatility of gasoline, fuel in GDI engines has sufficient time to premix and fewer locally fuel-rich regions are formed than in Compression Ignition Direct Injection (CIDI) engines, especially if the injection takes place long before top dead centre. So the traditional soot formation mechanism may not be applicable for GDI engines. The soot formation process in GDI engines has been widely investigated by optical