THE UNIVERSITY
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Faculty of Engineering, Computer and Mathematical Sciences

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# Performance of Petrodiesel and Biodiesel Fuelled Engines:

## A Fundamental Study of Physical and Chemical Effects

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# Nomenclature

Upper-Case Roman

| | |
|---|---|
| $A, B, C$ | Variable in Antoine equation |
| $C$ | Progress variable |
| $C_{st}$ | Progress variable at stoichiometric |
| $C_{\varepsilon 1}, C_{\varepsilon 2}, C_{\mu}$ | k – ε turbulence model constant |
| $C_{\chi}$ | Average scalar dissipation rate constant |
| $D$ | Mass diffusivity |
| $Da$ | Damköhler number |
| $D_e$ | Effective diffusivity |
| $E$ | Extinction limit |
| $E_a$ | Activation energy |
| $E_{\alpha 1}, E_{\alpha 2}$ | Semi-empirical soot model sub-model exponential terms |
| $I$ | Ignition limit |
| $K_A, K_B, K_T, K_Z$ | Nagle and Strickland-Constable oxidation sub-model constant |
| $L$ | Characteristic length |
| $L_{\alpha 1} \dots L_{\alpha 4}$ | Semi-empirical soot model sub-model linear terms |
| $M_1$ | First soot moment |
| $M_{c(s)}$ | Molecular weight of carbon atom |
| $N$ | Soot number density |
| $N_j$ | Soot number density for $j$ particles |
| $P$ | Pressure |
| $P_{H2O}$ | Partial pressure of water |
| $P_{O2}$ | Partial pressure of oxygen |
| $P_{OH}$ | Partial pressure of hydroxide |
| $P_v$ | Vapour pressure |
| $R$ | Universal gas constant |
| $R_1 \dots R_5$ | Leung et al. (1995) semi-empirical soot model source terms |
| $S$ | Soot surface area |
| $T$ | Local temperature |
| $T_a$ | Adiabatic flame temperature |
| $T_c$ | Critical temperature |
| $T_u$ | Unburnt fuel temperature |
| $V_u$ | Volume of domain |

| | |
|---|---|
| $W_{C2}$ | Molecular weight of $C_2$ |
| $Y_F$ | Mass fraction of fuel species |
| $Y_i$ | Mass fraction of species, i |
| $Y_{N2}$ | Mass fraction of nitrogen |
| $Y_{O2}$ | Mass fraction of oxygen |
| $Z$ | Mixture fraction |
| $Z_F$ | Mass fraction of all elements from fuel stream |
| $Z_i$ | Mixture fraction of species, i |
| $Z_O$ | Mass fraction of all elements from oxidiser stream |
| $Z_{st}$ | Stoichiometric mixture fraction |
| $\tilde{Z}''^2$ | Variance of mixture fraction |

## Lower-Case Roman

| | |
|---|---|
| $c_p$ | Specific heat capacity of species, i |
| $c$ | Specific heat |
| $d$ | Nozzle diameter |
| $d_c$ | Mean soot diameter |
| $f_m$ | Mass fraction |
| $f_v$ | Soot volume fraction |
| $h_g$ | Total gas-phase enthalpy per unit mass |
| $h_i$ | Specific enthalpy of species, i |
| $j_{i\alpha}$ | Diffusion mass flux of species, i |
| $k$ | Thermal conductivity |
| $k$ | Turbulent kinetic energy |
| $m_f$ | Mass of soot formed |
| $m_{fi}$ | Mass of fuel burnt |
| $m_j$ | Soot particle mass of $j$ particles |
| $m_{lt}$ | Mass of liquid fuel in domain |
| $m_o$ | Mass of soot oxidised |
| $m_s$ | Overall mass of soot |
| $\dot{q}_R$ | Power lost by radiation |
| $t$ | Time |
| $\boldsymbol{u}$ | Reynolds-averaged mean gas-phase velocity vector |
| $\dot{w}_l$ | Chemical kinetic source term |

| $x_{pen}$ | Vapour-phase penetration |
|---|---|

## Upper-Case Greek

| $\alpha$ | Fenimore and Jones oxidation rate parameter |
|---|---|
| $\Delta P$ | Injection pressure |
| $\phi$ | Scalar variable |

## Lower-Case Greek

| $\alpha_1 \ldots \alpha_4$ | Semi-empirical soot equation mass source terms |
|---|---|
| $\beta_1, \beta_2$ | Semi-empirical soot equation number source terms |
| $\gamma$ | Surface tension |
| $\lambda_e$ | Effective thermal conductivity |
| $\lambda_i$ | Thermal conductivity of species, i |
| $\lambda_l$ | Laminar thermal conductivity |
| $\lambda_t$ | Turbulent thermal conductivity |
| $\mu_e$ | Effective viscosity |
| $\mu_l$ | Laminar viscosity |
| $\mu_t$ | Turbulent viscosity |
| $v$ | Kinematic viscosity |
| $v_F$ | Reaction coefficients of fuel species |
| $v_{N2}$ | Reaction coefficients of nitrogen |
| $v_{O2}$ | Reaction coefficients of oxygen |
| $v_T$ | Turbulent viscosity |
| $\rho$ | Density |
| $\rho_a$ | Ambient density |
| $\rho_{c(s)}$ | Soot density |
| $\rho_g$ | Gas-phase density |
| $\rho_i$ | Partial density of species, i |
| $\rho_l$ | Fuel density |
| $\rho y_s$ | Species density of soot |
| $\sigma_k, \sigma_\varepsilon$ | $k - \varepsilon$ turbulence model constant |
| $\tau$ | Turbulent stress tensor |
| $\chi$ | Scalar dissipation rate |
| $\chi_{ext}$ | Extinction scalar dissipation rate |

| | |
|---|---|
| $\chi_{ign}$ | Ignition scalar dissipation rate |
| $\tilde{\chi}$ | Average scalar dissipation rate |
| $\omega$ | Angular velocity |
| $\widetilde{\omega}_{\varphi}$ | Fávre-averaged source terms |
| $\dot{\omega}_{\varphi}$ | Instantaneous source terms |

## Symbols

| | |
|---|---|
| *erf* | Error function |

## Abbreviations

| | |
|---|---|
| *A1* | Benzene |
| *A2* | Naphthalene |
| *A3* | Phenanthrene |
| *A4* | Pyrene |
| *ASI* | After start of injection |
| *CI* | Compression-ignition |
| *CYA* | Cai, Yen and Abraham |
| *DLFC* | Diffusion Laminar Flamelet Code |
| *EIA* | U.S. Energy Information Administration |
| *FAME* | Fatty acid methyl ester |
| *HACA* | Hydrogen-abstraction carbon-addition |
| *HEP* | Heptane |
| *JSR* | Jet-stirred reactor |
| *LHV* | Lower heating value |
| *LLJ* | Leung, Lindstedt, and Jones |
| *LLNL* | Lawrence Livermore National Laboratory |
| *MB* | Methyl butanoate |
| *MD* | Methyl decanoate |
| *MD9D* | Methyl-9-decenoate |
| *OppDif* | Opposed-flow diffusion flame |
| *PAH* | Polycyclic aromatic hydrocarbons |
| *PDF* | Probability density function |
| *PPM* | Parts per million |
| *PSR* | Perfectly-stirred reactor |

| | |
|---|---|
| *RANS* | Reynolds-averaged Navier-Stokes |
| *REC* | Reciprocating Engine Code |
| *RXN* | Reaction |
| *SMD* | Sauter-mean diameter |
| *TBS* | Ternary biodiesel surrogate |

# Abstract

In this work, biodiesel and petrodiesel combustion is studied under conditions that represent those in an engine at top-dead-centre. The primary focus of this study is on improving the understanding of biodiesel feedstock properties on spray structure, understanding the effect of strain on soot formation in biodiesel and petrodiesel combustion using a kinetics-based soot model, developing a simplified soot model that can model soot formation in both biodiesel and petrodiesel combustion, and applying the model to study soot formation in sprays. The differences in feedstock properties primarily affect the liquid phase penetration. It is shown that liquid penetration is influenced by entrainment rate, vapour pressure, and the average droplet size, in decreasing order of influence. The vapour-phase penetration and mixture fraction distribution in the sprays are not significantly influenced by the changes in feedstock properties.

Kinetic mechanisms for the oxidation of surrogate fuels for biodiesel and diesel and for soot formation are employed in the study. A one-dimensional flamelet code is employed to investigate the response of the soot formation to changes in scalar dissipation rate. The soot formation in biodiesel combustion is found to be more sensitive to changes in scalar dissipation rate. This suggests that increasing turbulence in a biodiesel-fuelled engine is likely to have a greater impact on soot emissions than in a petrodiesel-fuelled engine. Through a reaction pathway analysis, it is found that the differences in soot are on account of differences in the concentration of the aromatic species. Critical kinetic pathways and important species responsible for soot formation are identified for the fuels.

Having identified the critical species and pathways, a semi-empirical two-equation soot model is developed to model soot in both hydrocarbon diesel and biodiesel combustion. Results from the kinetic soot formation model are employed to calibrate the constants of the semi-empirical model. To the best knowledge of the author, this is the first soot model formulated that can model soot formation in the combustion of both fuels. The semi-empirical model is implemented in an in-house Reynolds-averaged Navier Stokes (RANS) multi-dimensional spray code and employed to predict soot in biodiesel and diesel sprays. The computed spray results are compared with available measurements in the literature. Compared to the performance of another well-validated semi-empirical two-equation soot model, the soot model developed in this work is shown to better predict soot in both biodiesel and diesel sprays.

# Declaration of Originality

This work contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution to Gary Cai. To the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text.

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*Signed*

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Gary Cai