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Performance of Petrodiesel and
Biodiesel Fuelled Engines:
A Fundamental Study of Physical and Chemical Effects

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Table of Contents

Nomenclature	ix
Abstract	xiv
Declaration of Originality	xv
1 Introduction	1
1.1 Objectives.....	8
1.2 Thesis Outline	8
2 Literature Review	10
2.1 Introduction.....	10
2.2 Non-reacting/Reacting Diesel Jets	10
2.3 Modelling of Petrodiesel and Biodiesel	14
2.3.1 <i>Surrogates for Petrodiesel</i>	15
2.3.2 <i>Surrogates for Biodiesel</i>	16
2.4 Pollutant Formation Pathways	18
2.4.1 <i>NO</i>	18
2.4.2 <i>Soot</i>	20
2.5 Biodiesel Fuel Research.....	26
2.6 Summary	31
3 Computational Methods	32
3.1 Introduction.....	32
3.2 Flamelet Model	32
3.2.1 <i>Theory</i>	32
3.2.2 <i>Governing Equations</i>	33
3.3 Multi-Dimensional Engine Model	36
3.3.1 <i>Gas-phase Governing Equations</i>	37
3.3.2 <i>Turbulence Model</i>	39
3.3.3 <i>Turbulence-Flame Interaction Model</i>	39
3.3.4 <i>Pollutant Modelling</i>	40
3.3.5 <i>Residence Time Tracking</i>	41
4 Biodiesel Feedstock Effects on Spray Structure	42
4.1 Introduction.....	42
4.2 Feedstock Selection.....	42
4.2.1 <i>Molar Mass, Critical Temperature, and Specific Heat</i>	43

4.2.2	<i>Vapour Pressure</i>	44
4.2.3	<i>Thermal conductivity</i>	45
4.2.4	<i>Liquid Density</i>	45
4.2.5	<i>Viscosity</i>	46
4.2.6	<i>Surface Tension</i>	46
4.2.7	<i>Sauter Mean Diameter</i>	47
4.3	Results and Discussion.....	47
4.3.1	<i>Liquid-phase Penetration</i>	47
4.3.2	<i>Gas-phase Penetration</i>	51
4.3.3	<i>Mixture Fraction Distribution</i>	52
4.4	Summary	53
5	Limit Phenomena	55
5.1	Introduction	55
5.2	Background	55
5.3	Influence of Strain on Pollutants.....	57
5.4	Summary and Conclusions.....	61
6	Soot Formation Reaction Pathway Analysis	63
6.1	Introduction	63
6.2	304-Species TBS Mechanism	63
6.3	Reaction Pathway Analysis.....	65
6.4	Summary and Conclusions.....	70
7	Two-Equation Soot Model Formulation	71
7.1	Introduction	71
7.2	General Formulation of Two-Equation Soot Models.....	71
7.3	Computational Method.....	72
7.4	The Proposed Two Equation Soot Model	75
7.4.1	<i>Soot Inception</i>	76
7.4.2	<i>Surface Growth</i>	76
7.4.3	<i>Coagulation</i>	77
7.4.4	<i>Oxidation by O₂</i>	77
7.4.5	<i>Oxidation by OH</i>	78
7.5	Sensitivity Analysis of the Model	78
7.5.1	<i>Addressing Soot Oxidation in Lean Mixtures</i>	81
7.6	Conclusion and Summary	84

8	Modelling Diesel Sprays with Two-Equation Soot Model	85
8.1	Introduction	85
8.2	Computational Conditions	85
8.3	Other Soot Models Considered	86
8.3.1	<i>Leung et al Two-Equation Soot Model</i>	86
8.3.2	<i>Kinetics-based Soot Model</i>	87
8.4	Results and Discussion.....	88
8.5	Summary and Conclusions.....	91
9	Biodiesel and Diesel Sprays	93
9.1	Introduction	93
9.2	Computational Conditions	93
9.3	Results and Discussion.....	94
9.4	Reacting Jet	97
9.5	Summary and Conclusions.....	99
10	Summary, Conclusions, and Future Work	101
10.1	Summary and Conclusions	101
10.2	Future Work	104
	References.....	106
	Appendix A: Combustion Characteristics of Surrogate Fuels	120
	Appendix B: Extra Species in the 304-Species TBS Mechanism.....	124
	Biography	125
	List of Publications	126

List of Tables

Table 1.1: Properties of #2 diesel compared with those of biodiesel.	5
Table 1.2: Fatty acid methyl ester composition of biodiesel fuels (Goering, 1982). Given in weight %	6
Table 4.1: Each of the seven feedstocks approximated (weight %) to be consisting of the three major FAMES.	44
Table 4.2: Some of the properties employed in the spray calculations.	50
Table 5.1: Ignition and extinction limits for the fuel surrogates.	57
Table 5.2: Soot formation characteristics for HEP253, TBS214 and TBS304.....	60
Table 5.3: NO formation characteristics for HEP253, TBS214 and TBS304.	61
Table 6.1: Reaction pathway analysis for the formation of A1	69
Table 7.1: Values of constants selected for sensitivity study.	78
Table 7.2: Model constants.....	83
Table 8.1: Computational conditions for the n-heptane spray. Parameter changed in each case in bold and underlined.	86
Table 9.1: Constant-volume chamber conditions for the reacting jet study.	94
Table A.1: Adiabatic flame temperature (K) at 1 atm for reactant temperature of 298 K. ...	120
Table A.2: Adiabatic flame temperature (K) at 40 atm for reactant temperature of 1000 K.	121

List of Figures

Figure 1.1: World crude oil consumption compared to production (EIA, 2013).	1
Figure 1.2: Extraction of various fuels from crude oil (Chevron, 1998).	2
Figure 1.3: World crude oil consumption by sector (IEA, 2014).	3
Figure 1.4: World transportation consumption based on fuel (EIA, 2012).	3
Figure 1.5: Transesterification process of a vegetable oil feedstock to biodiesel.	4
Figure 1.6: Chemical structure of oleic acid, $C_{18}H_{34}O_2$	4
Figure 2.1: Conceptual drawing of a non-reacting diesel spray	11
Figure 2.2: Non-dimensional axial penetration with respect to non-dimensional time for vaporising and non-vaporising sprays at different ambient densities (Bajaj et al., 2011).	12
Figure 2.3: Ignition and extinction S-curve.	13
Figure 2.4: Conceptual illustration of a combustng diesel-jet (Dec, 1997).	14
Figure 2.5: PAH build-up via the hydrogen-abstraction carbon-addition mechanism (Frenklach and Wang, 1994).	20
Figure 2.6: Stages of soot formation and growth (Bockhorn, 1994).	21
Figure 2.7: Simulated and measured PAH concentration of a turbulent flame (Kohler et al., 2012).	26
Figure 2.8: Primary oxidation pathway of a typical biodiesel fuel (Herbinet et al., 2008).	27
Figure 3.1: Conceptual illustration of flamelets.	33
Figure 3.2: Conceptual drawing of diffusion flamelets.	35
Figure 3.3: Computational grid used in REC.	37
Figure 4.1: Biodiesel production by region.	42
Figure 4.2: Critical Temperature (K) with respect to FAME chain length (Sales-Cruz et al., 2010).	43
Figure 4.3: Log-scale vapour pressure (kPa) with respect to $(1/T)$. Data taken from Yuan and Hansen (2005).	44
Figure 4.4: Thermal conductivity for FAMEs plotted against temperature (Annaken, 2011).	45
Figure 4.5: Liquid density of FAMEs with respect to temperature (Annaken, 2011).	45
Figure 4.6: Dynamic viscosity of FAMEs with respect to temperature (Annaken, 2011).	46
Figure 4.7: Surface tension of each FAME with respect to temperature (Annaken, 2011).	47
Figure 4.8: Liquid penetration of the biodiesel fuels and the soybean-derived biodiesel measurement from Nerva et al. (2012). Ambient temperature of 900 K (a) above, 1000 K (b) below.	48

Figure 4.9: Vapour pressure of the biodiesel fuels. Vertical axis is in log-scale. Temperature equivalent ranges from 373.15 K to 3073.15 K. Vapour pressure (kPa) at selected temperatures (K) shown in the inset table, along with the mean and standard deviation.	50
Figure 4.10: Vapour penetration of the biodiesel fuels compared to the soybean-derived measurement from Nerva et al. (2012) and an analytical curve.	52
Figure 4.11: Mixture fraction contours of the biodiesel fuels at 4 ms after the start of injection. 900 K cases (a) above and 1000 K cases (b) below. Feedstocks: castor, corn, palm, rapeseed, soybean, sunflower and tallow represented by (1) to (7). Lower cut-off fo.....	53
Figure 5.1: Temperature evolution of a diesel surrogate, n-heptane, at (a) χ of 59 s^{-1} , and (b) χ of 1542 s^{-1}	56
Figure 5.2: Soot volume fraction rising continuously over time for the petrodiesel surrogate mechanism at a χ of 5 s^{-1}	58
Figure 5.3: Soot volume fraction at various χ for a) HEP253, and b) TBS214.	59
Figure 5.4: NO species concentration at various strain rates for a) HEP253 and b) TBS214.	61
Figure 6.1: Creation of a 214-species biodiesel mechanism.	64
Figure 6.2: Time evolution of soot volume fraction for TBS 214 and TBS304.	64
Figure 6.3: a) Soot volume fraction and b) NO concentration for the three fuel surrogates. ...	65
Figure 6.4: C ₂ H ₂ concentration for the three fuel surrogate mechanisms.	66
Figure 6.5: A1 concentration for the three fuel surrogate mechanisms.	66
Figure 6.6: Plots for temperature, soot volume fraction, and acetylene, A4 and A1 mass fraction.	67
Figure 6.7: Reaction pathway of critical species that affects the formation of A1.	70
Figure 7.1: Volume fraction of soot (a), and mass fraction of (b) A1, (c) C ₂ H ₂ , (d) C ₂ H ₃ in the diffusion flame.	74
Figure 7.2: Predicted soot volume fraction for varying values of $L\alpha_1$, $E\alpha_1$, $L\alpha_2$, $E\alpha_2$, $L\alpha_3$ and $L\alpha_4$ as listed in Table 2 are shown in (a)-(f), respectively. The line types are identified in (a).	79
Figure 7.3: Predicted soot volume fractions with the preliminary set of constants in the two-equation model compared with the predictions of the ABF model.	81
Figure 7.4: Soot volume fraction when (a) $L\alpha_3$ is increased for the diesel surrogate, (b) $L\alpha_2$ increased with a constant $L\alpha_3$, and (c) $L\alpha_4$ increased with a constant $L\alpha_2$ and $L\alpha_3$. (a2), (b2) and (c2) show zoomed region of $Z = 0 - 0.15$	82
Figure 7.5: Soot volume fraction predicted by the two-equation soot model compared to the ABF soot model for χ_{st} of a) 5/s and b) 10/s.	83

Figure 8.1: Temperature contours for the nine cases at 4 ms ASI with (a) – (i) representing Cases 1 – 9, respectively.....	89
Figure 8.2: Soot volume fraction contour for the nine cases at 4 ms ASI.....	89
Figure 8.3: Soot volume fraction with respect to axial distance at the centreline for Cases 1, 5, 6, and 9 at 4 ms ASI with (a) - (d) representing them, respectively. Soot is normalised in each case independently.....	90
Figure 8.4: Soot volume fraction comparison between measured data (a), ABF kinetics soot mechanism (b), CYA soot model (c), LLJ soot model (d). Cases 1, 5, 6, 7 and 9 are compared. Measured data is from Engine Combustion Network (www.sandia.gov/ecn/).	92
Figure 9.1: Non-reacting and reacting liquid penetration plotted against time. 900 K ambient (a,b) and 1000 K ambient (c,d). Non-reacting (a,c), reacting (b,d).	95
Figure 9.2: Spray penetration as a function of time when the spray tip is identified as the location where the mixture fraction is (a) 0.0025, and (b) 1E-6.	96
Figure 9.3: Mixture fraction contour plots of the computed non-reacting jets. Ambient temperature of 900 K is plotted above (a,b) and 1000 K below (c,d). Biodiesel cases left, diesel cases right. Stoichiometric mixture fraction is emphasised by thick line. Contour ranges from 0.0025 – 0.1.	97
Figure 9.4: Temperature contour plots of the computed reacting jets. Ambient temperature of 900 K is plotted above (a,b) and 1000 K below (c,d). Biodiesel cases left, diesel cases right. Temperature ranges from 1,900 – 2,300 K.....	98
Figure 9.5: Soot volume fraction contour plots of the computed reacting jets. Ambient temperature of 900 K is plotted above (a,b) and 1000 K below (c,d). Biodiesel cases left, diesel cases right.	98
Figure 9.6: Predicted (a) soot volume fraction compared to measured data (b). Proceeding downwards, sprays are: 1000 K diesel, 1000 K biodiesel, 900 K diesel, 900 K biodiesel. Measured data taken from work of Nerva et al. (2012).....	99
Figure A.1: Adiabatic flame temperature (K) at 1 atm and initial temperature of 298 K.	121
Figure A.2: Adiabatic flame temperature (K) at 40 atm and initial temperature of 1000 K. .	121
Figure A.3: S_L (cm/s) of the diesel and biodiesel fuel surrogates with respect to ϕ at 1 atm and initial temperature of 298 K.....	122
Figure A.4. S_L (cm/s) of the diesel and biodiesel fuel surrogates with respect to ϕ at 40 atm and initial temperature of 1000 K.....	123

Nomenclature

Upper-Case Roman

A, B, C	Variable in Antoine equation
C	Progress variable
C_{st}	Progress variable at stoichiometric
$C_{\epsilon 1}, C_{\epsilon 2}, C_{\mu}$	k – ϵ turbulence model constant
C_{χ}	Average scalar dissipation rate constant
D	Mass diffusivity
Da	Damköhler number
D_e	Effective diffusivity
E	Extinction limit
E_a	Activation energy
E_{a1}, E_{a2}	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
$L_{a1} \dots L_{a4}$	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_{H_2O}	Partial pressure of water
P_{O_2}	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_{C_2}	Molecular weight of C_2
Y_F	Mass fraction of fuel species
Y_i	Mass fraction of species, i
Y_{N_2}	Mass fraction of nitrogen
Y_{O_2}	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_{ia}	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
\mathbf{u}	Reynolds-averaged mean gas-phase velocity vector
\dot{w}_i	Chemical kinetic source term

Upper-Case Greek

α	Fenimore and Jones oxidation rate parameter
ΔP	Injection pressure
ϕ	Scalar variable

Lower-Case Greek

$\alpha_1 \dots \alpha_4$	Semi-empirical soot equation mass source terms
β_1, β_2	Semi-empirical soot equation number source terms
γ	Surface tension
λ_e	Effective thermal conductivity
λ_i	Thermal conductivity of species, i
λ_l	Laminar thermal conductivity
λ_t	Turbulent thermal conductivity
μ_e	Effective viscosity
μ_l	Laminar viscosity
μ_t	Turbulent viscosity
ν	Kinematic viscosity
ν_F	Reaction coefficients of fuel species
ν_{N_2}	Reaction coefficients of nitrogen
ν_{O_2}	Reaction coefficients of oxygen
ν_T	Turbulent viscosity
ρ	Density
ρ_a	Ambient density
$\rho_{c(s)}$	Soot density
ρ_g	Gas-phase density
ρ_i	Partial density of species, i
ρ_l	Fuel density
ρy_s	Species density of soot
$\sigma_k, \sigma_\epsilon$	k – ϵ turbulence model constant
τ	Turbulent stress tensor
χ	Scalar dissipation rate
χ_{ext}	Extinction scalar dissipation rate

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

Symbols

erf	Error function
-------	----------------

Abbreviations

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

<i>RANS</i>	Reynolds-averaged Navier-Stokes
<i>REC</i>	Reciprocating Engine Code
<i>RXN</i>	Reaction
<i>SMD</i>	Sauter-mean diameter
<i>TBS</i>	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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