FUEL DROPLETS’ HEATING AND EVAPORATION
AN APPLICATION TO BIODIESEL, DIESEL, GASOLINE AND THEIR BLENDS

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Outline

- Discrete Component (DC) model – Basic equations
- DC model – an application to biodiesel fuels
- Multi-dimensional quasi-discrete (MDQD) model – an application to diesel fuel
- MDQD model – an application to gasoline fuel
- MDQD model – an application to diesel-biodiesel fuel blends
- Current and future work
Discrete Component (DC) model

Basic equations

The heating of the droplet is described by the transient heat conduction equation:

\[ \frac{\partial T}{\partial t} = \kappa \left( \frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right) \]  

...(1)

\[ \kappa = \frac{\kappa_{\text{eff}}}{c_l \rho_l} \]  

& \kappa_{\text{eff}} \text{ is the effective thermal conductivity} \ (\kappa_{\text{eff}} = \chi k_l), \text{ taking into account the recirculation effect inside droplets:} \]

\[ \chi = 1.86 + 0.86 \tanh[2.225 \log_{10}(\text{Pe}_{d(l)}/30)], \]  

...(2)

The solution to Eq. (1) subject to the appropriate initial and boundary conditions:

\[ T(R,t_1) = \frac{1}{R} \sum_{n=1}^{\infty} \left\{ q_n \exp[-\kappa_R \lambda_n^2 t_1] - \frac{R_d^2}{\|v_n\|^2 \lambda_n^2} \frac{\sin \lambda_n}{\mu_0(0)} \exp[-\kappa_R \lambda_n^2 t] - \frac{R_d^2}{\|v_n\|^2 \lambda_n^4} \int_0^t \frac{d\mu_0(\tau)}{d\tau} \exp[-\kappa_R \lambda_n^2 (t - \tau)] d\tau \sin \left( \lambda_n \frac{R}{R_d} \right) + T_{\text{eff}}(t_1), \right\} \]  

...(3)

Effective Thermal Conductivity (ETC) model
The effect of internal recirculation on temperature distribution inside droplets moving with relative velocities (a) 0.2 m s\(^{-1}\), (b) 1 m s\(^{-1}\) and (c) 3 m s\(^{-1}\).

The time evolution of species mass fractions at any $R$ is derived from:

$$\frac{\partial Y_{li}}{\partial t} = D_{\text{eff}} \left( \frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right), \quad \ldots(4)$$

where $D_{\text{eff}}$ is the effective liquid species diffusivity ($D_{\text{eff}} = D_l \chi_Y$), taking into account the recirculation inside droplets:

$$\chi_Y = 1.86 + 0.86 \tanh \left[ 2.225 \log_{10} \left( \text{Re}_{d(l)} \text{Sc}_l / 30 \right) \right], \quad \ldots(5)$$

The solution to Eq. (4) subject the initial and boundary conditions:

$$Y_{li} = \epsilon_i + \frac{1}{R} \left\{ \left[ \exp \left[ D_{\text{eff}} \left( \frac{\lambda_0}{R_d} \right)^2 t \right] [q_{i0} - \epsilon_i Q_0] \sinh \left( \frac{\lambda_0}{R_d} R \right) \right] + \sum_{n=1}^{\infty} \left[ \exp \left[ -D_{\text{eff}} \left( \frac{\lambda_n}{R_d} \right)^2 t \right] [q_{in} - \epsilon_i Q_n] \sin \left( \frac{\lambda_n}{R_d} R \right) \right] \right\} \quad \ldots(6)$$

**Effective Diffusivity (ED) model**
DC model
Basic Equations

Evaporation rate for an isolated droplet

\[
\dot{m}_d = -2\pi R_d D_v \rho_g B_M \text{Sh}_{\text{iso}}
\]  \ ...(10)

\(\rho_g\) is assumed as the ambient gas density,

\(D_v\) is the binary diffusion coefficient of fuel vapour in air,

\(B_M = (Y_{v_s} - Y_{v\infty})/(1 - Y_{v_s})\) is the Spalding mass transfer number,

\(Y_{v_s} \& Y_{v\infty}\) are the vapour mass fractions near and away from the droplet surface, respectively,

\(Y_{v_s} = \sum_i Y_{vsi}\),

\(\text{Sh}_{\text{iso}}\) is the Sherwood number for an isolated evaporating droplet,

\[
\text{Sh}_{\text{iso}} = 2 \frac{\ln(1 + B_M)}{B_M} \left(1 + \frac{(1 + \text{Re}_d \text{Sc}_d)^{1/3} \max\left[1, \text{Re}_d^{0.077}\right] - 1}{2F(B_M)}\right)
\]  \ ...(11)
ED/ETC effects

Temperature

Mass fractions

$T$ and $Y_{li}$ versus $R/R_d$ at 3 time instants (0.02 ms, 0.3 ms and 0.5 ms), predicted by the ETC/ED model

$A$: alkylbenzene $C_{10}H_{14}$; $T$: tricycloalkane $C_{19}H_{34}$
DC Model
(an application to 19 biodiesel fuels)
Typical example of biodiesel fuel composition
# Composition of biodiesel fuels

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The time evolution of Palm Kernel Methyl Ester (PMK) droplet surface temperatures ($T_s$) and radii ($R_d$) predicted by ED/ETC, ID/ITC, using single- and multi-component models.
ED/ETC effects
Multi-dimensional quasi-discrete (MDQD) model
Quasi-Discrete Model*

\[ f_m(I) = C_m \frac{(I - \gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp \left[ - \left( \frac{I - \gamma}{\beta} \right) \right] \]

\[ f_m(n) = C_m(n_0, n_f) \frac{(M(n) - \gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp \left[ - \left( \frac{M(n) - \gamma}{\beta} \right) \right] \]

\[ \int_{n_0}^{n_f} f_m(n) \, dn = 1 \]

\[ M = 14n + 2 \]

Quasi-discrete model

- The model is based on replacing the large number of actual alkane components with a small number of quasi-components (QC)

- The model takes into account temperature gradient, diffusion of species and re-circulation inside droplets

![Graph showing distribution of carbon numbers in alkanes](image)

Alkanes

\[ C_n H_{2n+2} \]
Quasi-discrete model (basic equations)

\[ N_f \text{ quasi-components with carbon numbers} \]

\[ \bar{n}_j = \frac{\int_{n_{j-1}}^{n_j} n f_m(n) dn}{\int_{n_{j-1}}^{n_j} f_m(n) dn} \]

Molar fractions

\[ X_j = \int_{n_{j-1}}^{n_j} f_m(n) dn \quad \xrightarrow{\text{}} \quad \sum_{j=1}^{j=N_f} X_j = 1 \]

\[ \sum_{j=1}^{j=N_f} Y_j = 1 \]

\[ p^{\text{sat}}(n) = \exp \left( A(n) - \frac{B(n)}{T - C(n)} \right) \]
\[ L = \frac{R_u B(n) T^2}{M(n) (T - C(n))^2} \]

\[ A(n) = 6.318 n^{0.05091}, \quad B(n) = 1178 n^{0.4652}, \quad C(n) = 9.467 n^{0.9143}, \]
Realistic Diesel fuel composition

**MDQD model**

\[
\tilde{n}_{1m} = \frac{\sum_{n=n_1m}^{n=(\varphi_m+1)m} nX_{nm}}{\sum_{n=n_1m}^{n=(\varphi_m+1)m} X_{nm}},
\]

\[
\tilde{n}_{2m} = \frac{\sum_{n=n_1m}^{n=(2\varphi_m+2)m} nX_{nm}}{\sum_{n=n_1m}^{n=(2\varphi_m+2)m} X_{nm}},
\]

\[
\tilde{n}_{3m} = \frac{\sum_{n=n_1m}^{n=(3\varphi_m+3)m} nX_{nm}}{\sum_{n=n_1m}^{n=(3\varphi_m+3)m} X_{nm}},
\]

\[
\vdots
\]

\[
\tilde{n}_{lm} = \frac{\sum_{n=n_1m}^{n=(l\varphi_m+l)m} nX_{nm}}{\sum_{n=n_1m}^{n=(l\varphi_m+l)m} X_{nm}},
\]

\[
X_{1m} = \sum_{n=n_1m}^{n=(\varphi_m+1)m} X_{nm},
\]

\[
X_{2m} = \sum_{n=n_1m}^{n=(2\varphi_m+2)m} X_{nm},
\]

\[
X_{3m} = \sum_{n=n_1m}^{n=(3\varphi_m+3)m} X_{nm},
\]

\[
\vdots
\]

\[
X_{lm} = \sum_{n=n_1m}^{n=(l\varphi_m+l)m} X_{nm},
\]

\[
\sum_{j=1}^{N_f} X_j = 1
\]
Selection of component or quasi-components

$T_s$ and $R_d$ versus the number of components/quasi-components (C/QC) used for the approximation of a stationary Diesel fuel droplet at three time instants, 1 ms, 2 ms & 2.5 ms
The time evolution of surface temperatures ($T_s$) and radii ($R_d$) predicted by: 98, 15, 20 alkanes components/quasi-components, single-component, single alkane-component, and n-dodecane approximations.
The plot of CPU time, required for calculations of stationary droplet heating and evaporation for Intel Xeon (core duo) E8400, 2 GHz and 3 GB RAM for 1 μs time-step.
MDQD Model
(an application to gasoline fuel)
FACE gasoline fuel

\[
\bar{n}_{1m} = \frac{\sum_{n=n_1m}^{n_2m}(\varphi_{m+1})^m(nX_{nm})}{\sum_{n=n_1m}^{n_2m}(\varphi_{m+1})^m X_{nm}},
\]

\[
\bar{n}_{2m} = \frac{\sum_{n=n_2m}^{n_3m}(\varphi_{m+2})^m(nX_{nm})}{\sum_{n=n_2m}^{n_3m}(\varphi_{m+2})^m X_{nm}},
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\[
\bar{n}_{3m} = \frac{\sum_{n=n_3m}^{n_4m}(\varphi_{m+3})^m(nX_{nm})}{\sum_{n=n_3m}^{n_4m}(\varphi_{m+3})^m X_{nm}},
\]

\[
\bar{n}_{\ell m} = \frac{\sum_{n=n_{\ell m}}^{n_{\ell+1 m}}((\ell-1)\varphi_{m+\ell})^m(nX_{nm})}{\sum_{n=n_{\ell m}}^{n_{\ell+1 m}}((\ell-1)\varphi_{m+\ell})^m X_{nm}},
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Surface temperatures and radii

gasoline

$T_s (K)$

$R_d (\mu m)$

- $T_s (20)$
- $T_s (6)$
- $T_s (SI)$
- $T_s (IO)$
- $R_d (20)$
- $R_d (6)$
- $R_d (SI)$
- $R_d (IO)$

67%
The plot of CPU time, required for calculations of stationary droplet heating and evaporation for Intel Xeon (core duo) E8400, 2 GHz and 3 GB RAM for 1 μs time-step.
MDQD Model
(an application to diesel-biodiesel fuel blends)
The time step = 1 µs.

Workstation Specs. Z210, Intel core, 64-bit, 3.10 GHz and 8 GB RAM.
Conclusions

- The mono-component and ID/ITC models lead to errors in predicted biodiesel droplet evaporation time of up to about 26% compared with the multi-component and ED/ETC models.

- The approximations of realistic Diesel fuel by n-dodecane, or 20 alkane C/QC lead to large errors in predicted droplet evaporation time up to about 50% & 22%, respectively.

- The approximation of FACE gasoline fuel by iso-octane, or a single-component lead to large errors in predicted droplet evaporation time up to about 47% & 67%, respectively.

- Small fractions of biodiesel fuel (up to 5%) in diesel fuel blends have negligible effects on the evolutions of $T_s$ and $R_d$.

- The errors in the estimated $T_s$ and $R_d$ for biodiesel, using MDQD model, are negligible compared to those predicted using DC model.

- Using MDQD model resulted in a reduction of up to 96% in computational time compared to the CPU time using DC model.
In progress

- Experimental validation of the MDQD model.
- An application of the DC and MDQD models to mixtures of:
  - 22 biodiesel/diesel fuels,
  - Ethanol/gasoline fuels,
  - Ethanol-gasoline/Diesel fractions for diesel engines.
- Impacts of in-cylinder conditions on droplets lifetime, ignition, and emissions.
- Impacts of fuel blends and compositions on their surrogates’ formulation and ignition.
- Impacts of fuel blends and compositions on the spray formulation – implementing in-house code into ANSYS-fluent.
Preliminary data
Impact of ambient temperature on ethanol/gasoline blended fuel droplet lifetime

High ambient temperature (650 K)

Low ambient temperature (500 K)

High ambient pressure (20 bar)

Low ambient pressure (3 bar)
Impact of radiation temperature on ethanol/gasoline blended fuel droplet lifetime

\[ P_g = 9 \text{ bar}, \ T_g = 545 \text{ K} \]
### Compositions of 22 biodiesel fuels to blend with diesel fuel

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**Note:** The table represents the methyl esters and compositions of various fatty acids used in biodiesel production. Each row corresponds to a different plant fat or oil, and the columns represent the percentages of different fatty acids in the methyl esters. The values in the table are in percentage by weight.
Acknowledgement
The models and results were conducted in collaboration with Prof. S.S. Sazhin.

Thank you
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https://cumahara.coventry.ac.uk/user/view.php?id=39492