IMPROVEMENTS OF FUEL BLENDS AND AMBIENT CONDITIONS ON ETHANOL/GASOLINE DROPLET HEATING AND EVAPORATION

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The work has been conducted in collaboration with colleagues, Nawar Al-Esawi (Coventry University) and Sergei S. Sazhin (Brighton University).
Outline

- Basic equations
- Impact of corrected activity coefficient
- Impacts of ethanol/gasoline fuel blends
- Impacts of ambient temperature
- Impacts of ambient pressure
- Impacts of radiation
Basic equations
Temperature distribution

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

\[
\frac{\partial T}{\partial t} = \kappa \left( \frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right) \quad \text{...(1)}
\]

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

\[
\chi = 1.86 + 0.86 \tanh\left[2.225 \log_{10}\left(\text{Pe}_{d(l)}/30\right)\right], \quad \text{...(2)}
\]

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

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

\text{...(3)}
The droplet is assumed to be opaque and non-reflective (emissivity equal to 1). The following boundary condition is applied at its surface:

\[ k_{\text{eff}} \frac{\partial T}{\partial R} \bigg|_{R=R_d} = \rho L \frac{dR_d}{dt} + h(T_g - T_s) + \sigma T_{\text{rad}}^4 \]  

...(4)

\[ \sigma = 5.6703 \times 10^{-8} \text{ W m}^{-2}\text{K}^{-4} \]

In Eq. (3), the radiative effect will be taken into account in calculating the effective temperature:

\[ T_{\text{eff}} = T_g + \frac{\rho L dR_d}{h} + \frac{\sigma T_{\text{rad}}^4}{h} \]  

...(5)

The radiation flux emitted by the droplet \( \sigma T_d^4 \) to ambient gas is assumed to be negligible.
Species diffusion

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

$$\frac{\partial Y_{li}}{\partial t} = D_{\text{eff}} \left( \frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right),$$  \hspace{1cm} \text{...(6)}$$

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

$$\chi_l = 1.86 + 0.86 \tanh[2.225 \log_{10}(Re_{d(l)} Sc_l/30)],$$  \hspace{1cm} \text{...(7)}$$

The solution to Eq. (6) subject to initial and boundary conditions:

$$Y_{li} = \epsilon_i + \frac{1}{R} \left\{ \left[ \exp \left( D_{\text{eff}} \left( \frac{\lambda_0}{R_d} \right)^2 t \right) \right] \left[ q_{i0} - \epsilon_i Q_0 \right] \sinh \left( \frac{\lambda_0}{R_d} R \right) + \right\}$$

$$+ \sum_{n=1}^{\infty} \left[ \exp \left( -D_{\text{eff}} \left( \frac{\lambda_n}{R_d} \right)^2 t \right) \right] \left[ q_{in} - \epsilon_i Q_n \right] \sin \left( \frac{\lambda_n}{R_d} R \right) \right\}$$  \hspace{1cm} \text{...(8)}$$

Effective Diffusivity (ED) model
Evaporation rate for an isolated droplet

\[ \dot{m}_d = -2\pi R_d D_{\text{mix}} \rho_g B_M \text{Sh}_{\text{iso}} \]  

...(9)

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

\( D_{\text{mix}} \) is the mixed binary diffusion coefficient of blended fuel vapour in air, estimated using Sanchez-Clifton approach:

\[ D_{\text{mix}} = x_{\text{oct}} D_{\text{oct}} + x_{\text{eth}} D_{\text{eth}} \]  

...(10)

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

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

\[ Y_{vs} = \sum_i Y_{vsi}, \]

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

where \( x_{\text{oct}} \) and \( x_{\text{eth}} \) are the molar fractions of fuels.
Corrected activity coefficient ($\gamma$)

The universal quasi-chemical functional group activity-coefficient (UNIFAC) model is used to predict $\gamma$ to determine the vapor fractions ($x_{vi}$) in the vicinity of droplet, as:

$$x_{vi} = \frac{\gamma_i x_{lsi} p_{i}^{sat}}{p_g}$$  \hspace{1cm} \text{...(11)}

$x_{lsi}$ is molar fraction of component $i$ at the droplet surface, $p_{i}^{sat}$ is the saturated pressure of component $i$, & $p_g$ is the gas pressure. The UNIFAC can be presented as:

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R$$  \hspace{1cm} \text{...(12)}

$$\ln \gamma_i^C = \ln \frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{x_i} \sum_j x_j l_j, \ln \gamma_i^R = \sum_k v_k^i (\ln \Gamma_k - \ln \Gamma_k^i),$$

$$l_i = \frac{z}{2} (r_i - q_i) - (r_i - 1), \ Z = 10, \ \theta_i = \frac{q_i x_i}{\sum_j q_j x_j}, \ \Phi_i = \frac{r_i x_i}{\sum_j r_j x_j}, \ r_i = \sum_k v_k^i R_k, \ q_i = \sum_k v_k^i Q_k, \ \ln \Gamma_k = Q_k \left[ 1 - \ln \left( \sum_m \theta_m \psi_{mk} \right) - \sum_m \frac{\theta_m \psi_{km}}{\sum_n \theta_n \psi_{nm}} \right], \ \theta_m = \frac{Q_m x_m}{\sum_n Q_m x_m}, \ \text{and} \ \psi_{mn} = \exp \left( - \frac{a_{mn}}{T} \right).$$
Impact of activity coefficient on droplet lifetime prediction (diesel and gasoline fuels)
Gasoline fuel droplet

\[ R_{d0} = 12 \text{ µm} \]
\[ U_{d} = 24 \text{ m/s} \]
\[ T_{d} = 296 \text{ K} \]
\[ p_{g} = 9 \text{ bar} \]
\[ T_{g} = 545 \text{ K} \]

Gasoline

- UNIFAC activity coefficient
- Unity activity coefficient

2.6%
Diesel fuel droplet

$R_d^0 = 12.66 \, \mu m$

$U_d = 10 \, \text{m/s}$

$T_d = 360 \, \text{K}$,

$p_g = 30 \, \text{bar}$,

$T_g = 800 \, \text{K}$
Impact of ethanol/gasoline fuel blends
\[ R_{do} = 12 \text{ \( \mu \)m} \]
\[ U^d = 24 \text{ m/s} \]
\[ T^d_{do} = 296 \text{ K} \]
\[ p^d_{do} = 9 \text{ bar} \]
\[ T^g = 545 \text{ K} \]

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<tr>
<th>Blend</th>
<th>Lifetime (ms)</th>
<th>Diff*%</th>
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<tr>
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\[ \text{Diff}^* = \frac{\text{lifetime(\text{blend})} - \text{lifetime(E0)}}{\text{lifetime(E0)}} \times 100\% \]
Impact of ambient temperature (ethanol/gasoline fuels)
$p_g = 30 \text{ bar}$
$p_g = 3 \text{ bar}$
Impact of ambient pressure (ethanol/gasoline fuels)
$T_g = 650 \text{ K}$
$$T_g = 400 \text{ K}$$
Impact of radiative temperature (ethanol/gasoline fuels)
\( R_{d0} = 12 \, \text{µm} \)
\( U_d = 24 \, \text{m/s} \)
\( T_{d0} = 296 \, \text{K} \),
\( p_g = 9 \, \text{bar} \),
\( T_g = 545 \, \text{K} \)
<table>
<thead>
<tr>
<th>Blends</th>
<th>$T_{\text{rad}} = 1000$ K</th>
<th>$T_{\text{rad}} = 1500$ K</th>
<th>$T_{\text{rad}} = 2000$ K</th>
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</table>

$$\text{Diff} \% = \frac{\text{time}_{\text{no rad}} - \text{time}_{\text{w/ rad}}}{\text{time}_{\text{no rad}}}$$
Conclusions

- Without using the AC, droplet lifetimes are over-estimated by **4%** for diesel fuel, and **2.6%** for gasoline fuel.

- Less effective AC for gasoline droplets, compared to diesel fuel. The molecules in gasoline belong to one dominant group; i.e. the **interaction parameter** \( \approx 0 \).

- The droplet lifetime increases with higher ethanol fraction, with up to **34%** for E100 compared to E0.

- The predicted droplet surface temperature increases up to **24.3%** for E100, compared to E0.

- Increasing the radiative temperature, ambient pressure, or ambient temperature, usually leads to a **faster evaporation** of ethanol/gasoline droplets regardless of their blending fractions.

- At low ambient temperature (e.g. 400 K), increasing the ambient pressure can lead to **longer droplet** lifetimes.
Acknowledgement
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Thank you

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