Modelling of Diesel fuel droplet heating and evaporation: Kinetic and MD analysis

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Outline

- Engineering background
- Modelling of evaporation and condensation processes
  - Molecular dynamics (MD) simulation
  - Kinetic modelling
- Application to heating and evaporation of Diesel fuel droplet
- Energy balance analysis for high temperature ambient gas
- Summary
**Original ideas**

**Kinetic model**: the Boltzmann equation is solved in the kinetic region

\[
\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{F}{m} \frac{\partial f}{\partial v} = \frac{\partial f}{\partial t_{\text{collision}}}
\]

Plus, the **kinetic boundary condition (KBC)**: evaporation coefficient and velocity distribution

\[
f^{\text{out}} = \alpha f^e + (1 - \alpha) f^r
\]

\[
\frac{\alpha}{2} \geq 1
\]

\[
f^{\text{out}} \approx f^M
\]

**Discover** the evaporation coefficient and velocity distribution using **MD** technique.

(Xie, Sazhin & Cao, 2012)
MD simulation: \textit{equilibrium simulation}

**OPLS** (Optimised Potential for Liquid simulation)

**Constant - NVT ensemble**

Number of molecules:
\[ N = 720 \quad (N_x = 5, \quad N_y = 12 \quad \text{and} \quad N_z = 12) \]

Simulation box length:
\[ L_x \times L_y \times L_z = 25.25 \text{ nm} \times 6.48 \text{ nm} \times 6.48 \text{ nm} \]

Liquid temperature: \[ T_l = 500 \text{ K} \]

Periodic boundary condition (PBC) used in all directions

(Molecular structure of \textit{n}-dodecane (\textit{C}_{12}\textit{H}_{26})

(Xie, Sazhin & Cao, 2011; Cao, Xie & Sazhin, 2011)
velocity distribution and condensation coefficient

Velocity component normal to the vapour-liquid interface

Condensation coefficient versus liquid temperature

Velocity components parallel to the vapour-liquid interface

Distributions for all leaving molecules, evaporated and reflected

(Xie, Sazhin & Cao, 2012; Xie, Sazhin & Cao, 2011)
Revised kinetic boundary condition: $f^{out} = \alpha f^e + (1 - \alpha) f^r$

\[
\alpha = \alpha (T_L)
\]

\[
F^e_x = \frac{\alpha_e F^M_x}{\bar{\alpha}_e} = \frac{1 - \beta \exp(-E_x/2k_BT_L)}{1 - \beta/2} \left( \frac{m}{2\pi k_BT_L} \right)^{1/2} \exp \left( -\frac{E_x}{k_BT_L} \right)
\]

\[
F^r_x = \frac{1 - \alpha_e}{1 - \bar{\alpha}_e} F^M_x = \frac{1 - \alpha + \alpha \beta \exp(-E_x/2k_BT_L)}{1 - \alpha + \alpha \beta/2} \left( \frac{m}{2\pi k_BT_L} \right)^{1/2} \exp \left( -\frac{E_x}{k_BT_L} \right)
\]

(Xie, Sazhin & Cao, 2012)

**Kinetic modelling**

- Solve the **Boltzmann equation** in the kinetic region

\[
\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{F}{m} \frac{\partial f}{\partial v} = \frac{\partial f}{\partial t_{collision}}
\]

- The **inelastic collisions** is taken into account

- The **internal degrees of freedom** are considered
Inelastic collision model

Binary collision rules:

- The total number of degrees of freedom of each molecule $N_{total} = 3_{\text{translational}} + (N-3)_{\text{internal}}$

- One dimension in the $N$-dimensional space describes one of these degrees of freedom

- The energies of each molecule are redistributed between the degrees of freedom during the collisions and the total energy is conserved

(Shishkova, Sazhin & Xie, 2013)
Application: heating and evaporation of fuel droplet

Initial parameters:

\[ P_0 = 30 \text{ bar} \]
\[ T_{g0} = 1,500 \text{ K} \]
\[ T_s = 300 \text{ K} \]
\[ R_0 = 5 \mu m \]

(1) Hydrodynamic ITC model
(2) Kinetic ITC model without inelastic collision and with unity $\alpha$
(3) Kinetic ITC model with inelastic collision and unity $\alpha$
(4) Kinetic ITC model with inelastic collision and non-unity $\alpha$

(Sazhin, Xie & Shishkova, 2013)
High ambient gas temperature case

In most cases, the mass rate of a stationary droplet is given by

$$\dot{m}_d = -4\pi R_d D_g \rho_{total} \ln (1 + B_M)$$

**Limitations:**
- Mixture density is independent on the distance from the droplet surface
- Surface temperature is low
- Partial pressure of vapour is much less than the that of air

Moreover, it is not the case when $T_s$ approaches to or exceeds $T_B$.

The analysis of energy balance equation is an alternative:

$$4\pi R^2 k_g \frac{dT}{dR} = -\dot{m}_d c_{pv}(T - T_s) - \dot{m}_d L(T_s) + |\dot{q}_d|$$

And it can be rearranged to

$$4\pi k_g \frac{dT}{c_{pv}(T - T_s) + L(T_s) - (|\dot{q}_d|/\dot{m}_d)} = -\frac{\dot{m}_d dR}{R^2}.$$
A novel expression for mass rate:

\[
\dot{m}_d = -\frac{4\pi k_g R_d}{c_{pv}} \ln(1 + B_T)
\]

where, \(B_T = \frac{c_{pv}(T_g - T_s)}{L(T_s) - (|\dot{q}_d|/\dot{m}_d)}\) (Spalding heat transfer number)

and \(|\dot{q}_d| = 4\pi R_d^2 k_l \frac{\partial T}{\partial R}\bigg|_{R=R_d-0}\) (Heat rate at the droplet surface)

The solution to the heat conduction equation:

\[
T(R, t) = \frac{R_d}{R} \sum_{n=1}^{\infty} \left\{ q_n \exp \left[-\kappa_R \lambda_n^2 t\right] - \frac{\sin \lambda_n}{\| v_n \|^2} \frac{\mu_0(0)}{\lambda_n} \exp \left[-\kappa_R \lambda_n^2 t\right] - \sin \lambda_n \right\} \sin \left[\lambda_n \left(\frac{R}{R_d}\right)\right] + T_{\text{eff}}(t)
\]
The analytical solution to the heat rate:

\[
\frac{\partial T(R, t)}{\partial R} \bigg|_{R=R_d-0} = \frac{1}{R_d} \sum_{n=1}^{\infty} \left\{ q_n \exp \left[ -\kappa_R \lambda_n^2 t \right] - \frac{\sin \lambda_n}{\| v_n \|^2 \lambda_n^2} \mu_0(0) \exp \left[ -\kappa_R \lambda_n^2 t \right] - \right.

- \frac{\sin \lambda_n}{\| v_n \|^2 \lambda_n^2} \int_0^t \frac{d\mu_0(\tau)}{d\tau} \exp \left[ -\kappa_R \lambda_n^2 (t - \tau) \right] d\tau \right\} \left[ -\sin \lambda_n + \lambda_n \cos \lambda_n \right]

= \frac{1}{R_d} \sum_{n=1}^{\infty} \left\{ q_n \exp \left[ -\kappa_R \lambda_n^2 t \right] - \frac{\sin \lambda_n}{\| v_n \|^2 \lambda_n^2} \mu_0(0) \exp \left[ -\kappa_R \lambda_n^2 t \right] - \right.

- \frac{\sin \lambda_n}{\| v_n \|^2 \lambda_n^2} \int_0^t \frac{d\mu_0(\tau)}{d\tau} \exp \left[ -\kappa_R \lambda_n^2 (t - \tau) \right] d\tau \right\} \left[ -1 - h_0 \right] \sin \lambda_n.

\]

The analytical solution to the heat rate:

\[
|\dot{q}_d| = 4\pi R_d k_i \sum_{n=1}^{\infty} \left\{ q_n \exp \left[ -\kappa_R \lambda_n^2 t \right] - \frac{\sin \lambda_n}{\| v_n \|^2 \lambda_n^2} \mu_0(0) \exp \left[ -\kappa_R \lambda_n^2 t \right] - \right.

- \frac{\sin \lambda_n}{\| v_n \|^2 \lambda_n^2} \int_0^t \frac{d\mu_0(\tau)}{d\tau} \exp \left[ -\kappa_R \lambda_n^2 (t - \tau) \right] d\tau \right\} \left[ -1 - h_0 \right] \sin \lambda_n.

\]
Initial parameters:

\[ P_0 = 30 \text{ bar} \]
\[ T_{g0} = 1,500 \text{ K} \]
\[ T_s = 300 \text{ K} \]
\[ R_0 = 5 \mu\text{m} \]

<table>
<thead>
<tr>
<th>Model</th>
<th>Previous ETC</th>
<th>Present ETC</th>
<th>Previous-kinetic</th>
<th>Present-kinetic</th>
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<tbody>
<tr>
<td>( T_s (K) )</td>
<td>618.64</td>
<td>619.58</td>
<td>626.47</td>
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<td>( t_e (ms) )</td>
<td>0.2422</td>
<td>0.2488</td>
<td>0.2419</td>
<td>0.2481</td>
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</tbody>
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Summary

- **Molecular dynamics simulations** of evaporation and condensation
  - evaporation/condensation coefficient
  - velocity distribution functions

- **Kinetic modelling** of evaporation in the kinetic region, taking into account inelastic collisions

- Application to the heating and evaporation of *Diesel fuel droplet* in engine-like conditions

- **Energy balance analysis** for high ambient gas temperature
References


