# Kinetic and molecular dynamics modelling of diesel fuel droplet heating and evaporation

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CAE WORKSHOP

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# Outline

- Background
- Molecular dynamics (MD) simulation of evaporation and condensation
- Kinetic modelling of evaporation and condensation
- Application: heating and evaporation of diesel fuel droplet
- Summary

# Original ideas

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

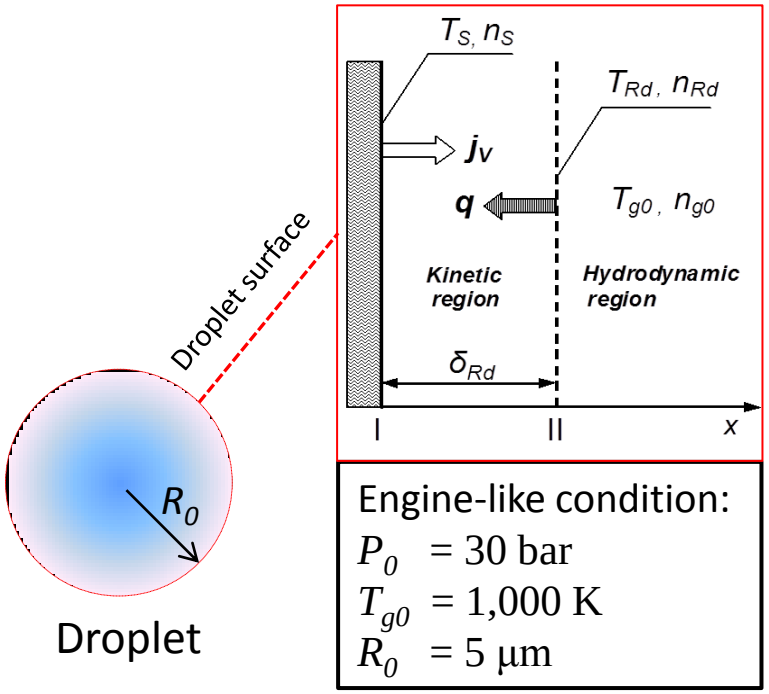
$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + \frac{F}{m}\frac{\partial f}{\partial v} = \frac{\partial f}{\partial t}_{collision}$$

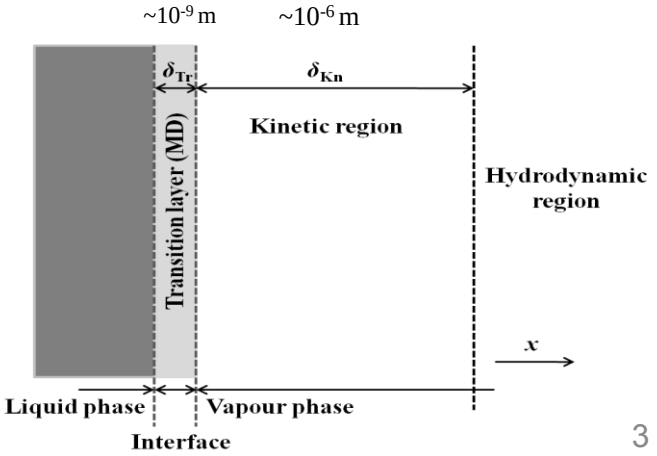
Plus, the **kinetic boundary condition** (***KBC***):
evaporation coefficient and velocity distribution

$$f^{out} = \alpha f^{e} + (1-\alpha) f^{r}$$

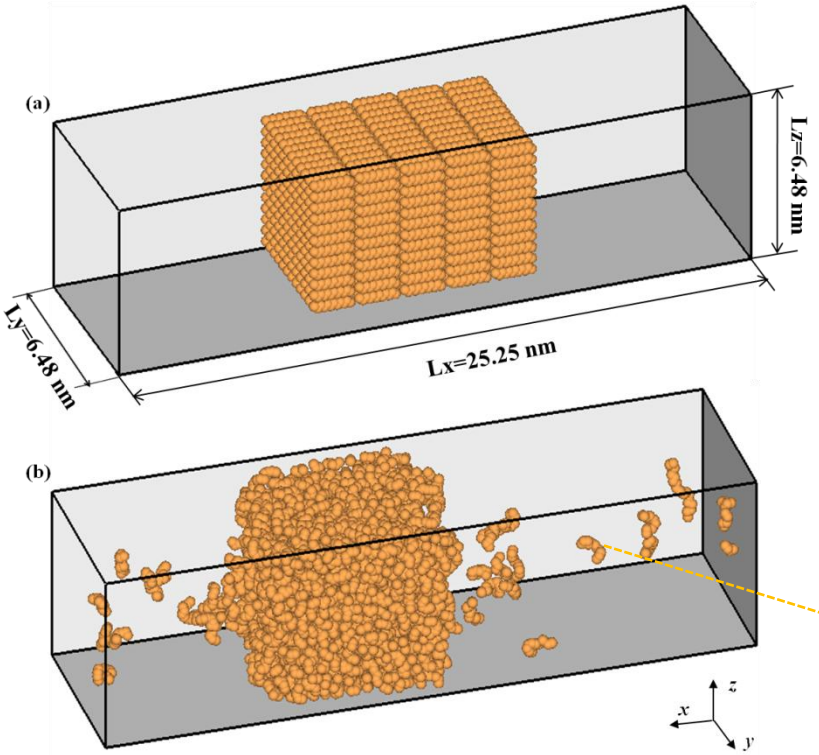
$$\alpha \stackrel{?}{=} 1$$
$$f^{out} \stackrel{?}{=} f^{M}$$

***Discover*** the evaporation coefficient and velocity distribution in terms of MD technique.



# MD simulation: *equilibrium simulation*




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

**Constant - *NVT* ensemble**

Number of molecules:

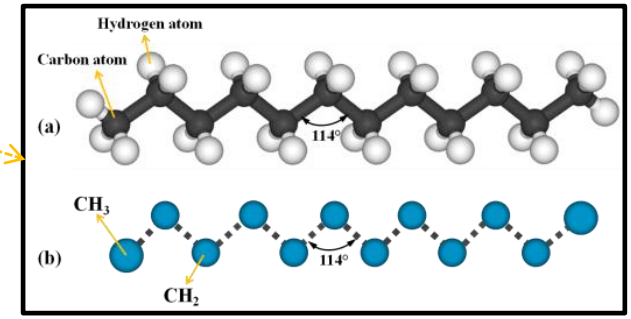
N= 720 ($N_x$= 5, $N_y$= 12 and $N_z$= 12)

Simulation box length:

$L_x$ x $L_y$ x $L_z$=25.25 nm x 6.48 nm x 6.48 nm

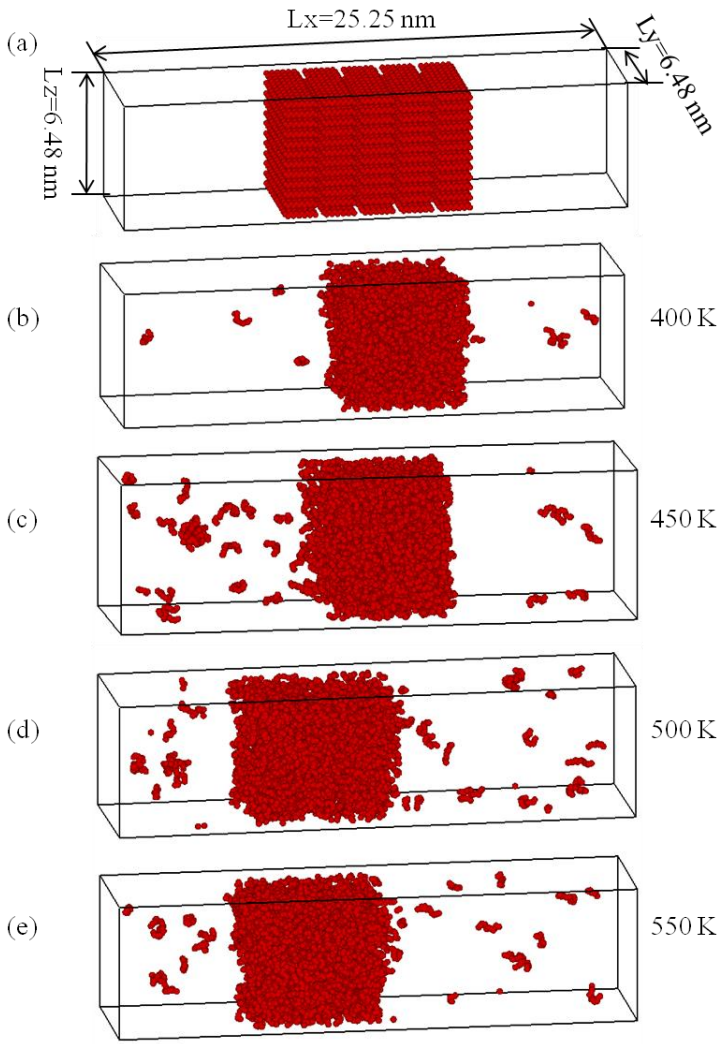
Liquid temperature: $T_l$ = 500K

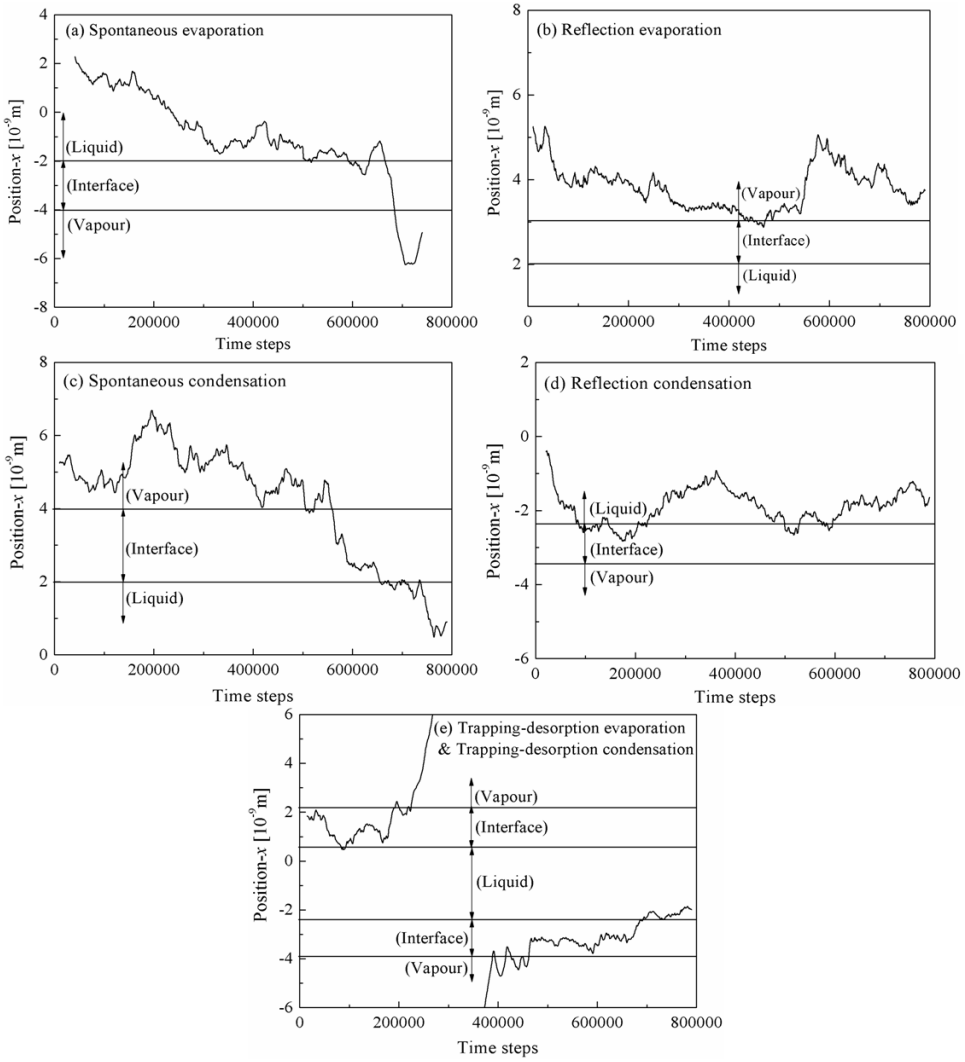
Periodic boundary condition (***PBC***) used in all directions



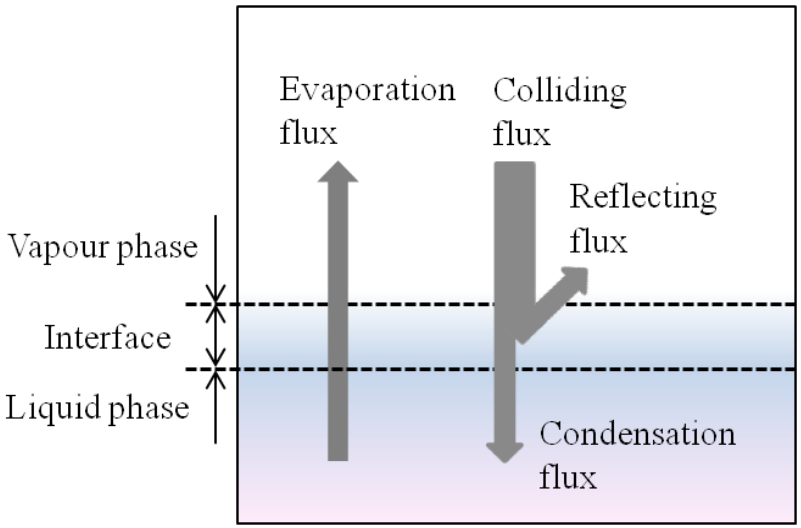

Molecular structure of *n*-dodecane ($C_{12}H_{26}$)

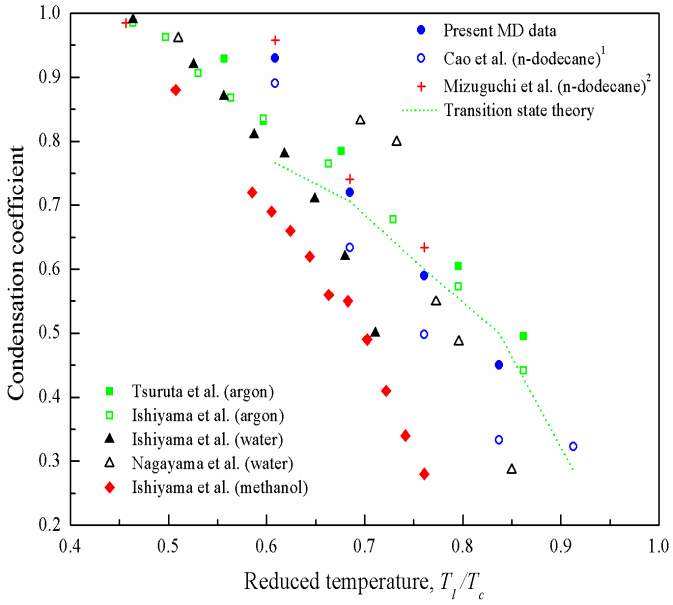
# Results and analysis: ***molecular behaviours***



# Results and analysis: ***condensation coefficient***



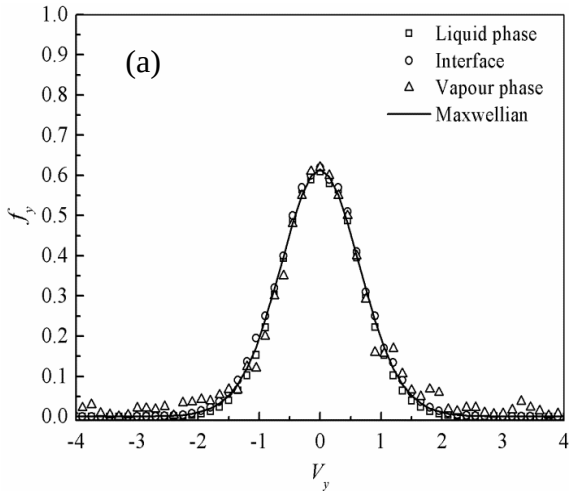



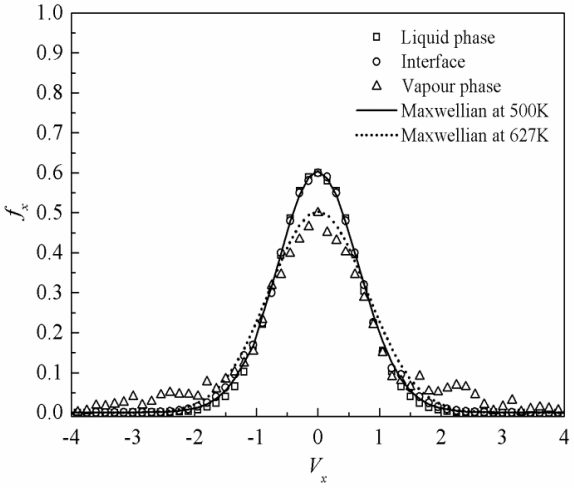

$$\alpha_e = \frac{Evaporation\ flux}{Outgoing\ flux}$$

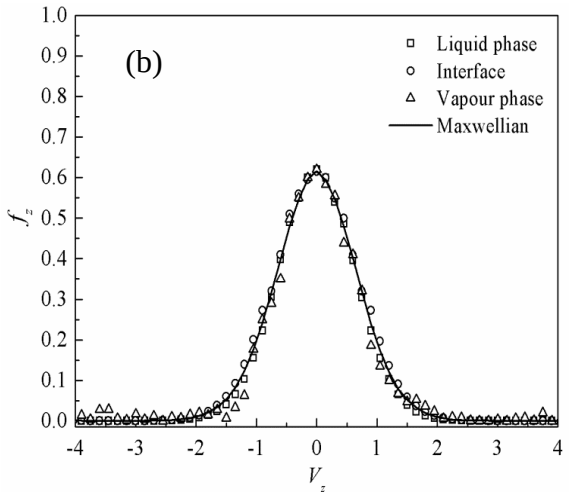
$$\alpha_c = \frac{Condensation\ flux}{Colliding\ flux}$$

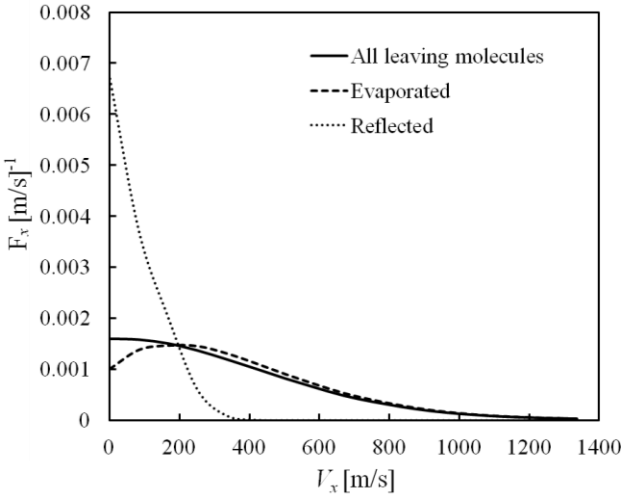
$$\alpha_e = \alpha_c \text{ (in equilibrium state)}$$

# Results and analysis: ***velocity distribution***



**Revised** kinetic boundary condition: $\boldsymbol{f^{out} = \alpha f^{e} + (1-\alpha) f^{r}}$

$$\alpha = \alpha\,(T_L)$$

$$F_x^e = \frac{\alpha_e}{\bar{\alpha}_e} F_x^M = \frac{1-\beta exp(-E_x/2k_BT_l)}{1-\beta/2}\left(\frac{m}{2\pi k_BT_l}\right)^{1/2} exp\left(-\frac{E_x}{k_BT_l}\right)$$

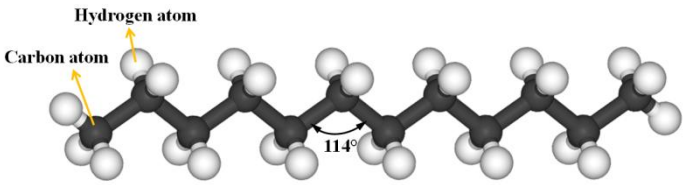
$$F_x^r = \frac{1-\alpha_e}{1-\bar{\alpha}_e} F_x^M = \frac{1-\alpha+\alpha\beta exp(-E_x/2k_BT_l)}{1-\alpha+\alpha\,\beta/2}\left(\frac{m}{2\pi k_BT_l}\right)^{1/2} exp\left(-\frac{E_x}{k_BT_l}\right)$$

## Kinetic modelling

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

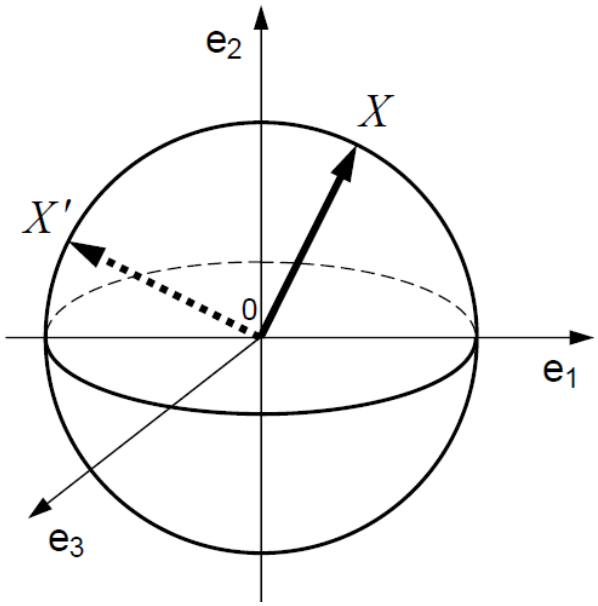
$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + \frac{F}{m}\frac{\partial f}{\partial v} = \frac{\partial f}{\partial t}_{collision}$$

- The **inelastic collisions** is taken into account
- The **internal degrees of freedom** are considered




Chain-like molecule ($C_{12}H_{26}$)

# Inelastic collision model



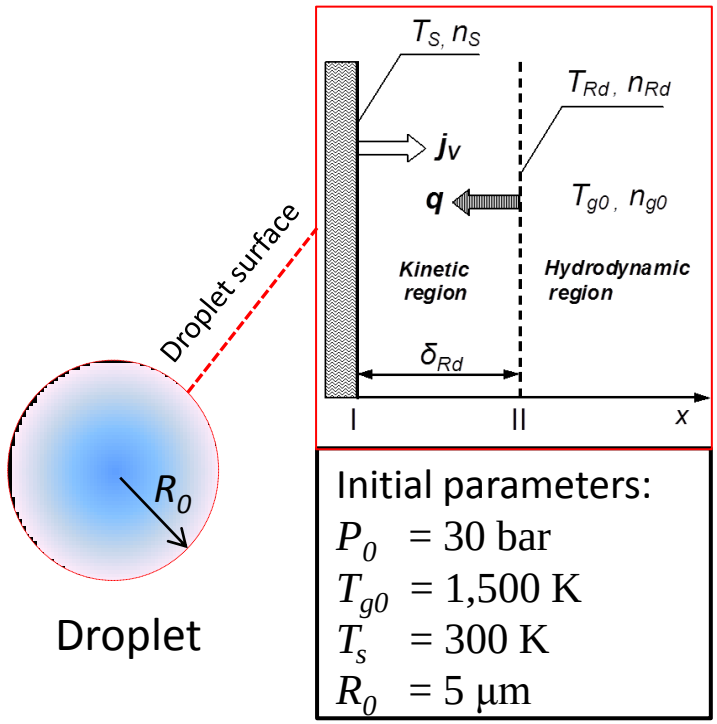

## Binary collision rules:

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

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

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

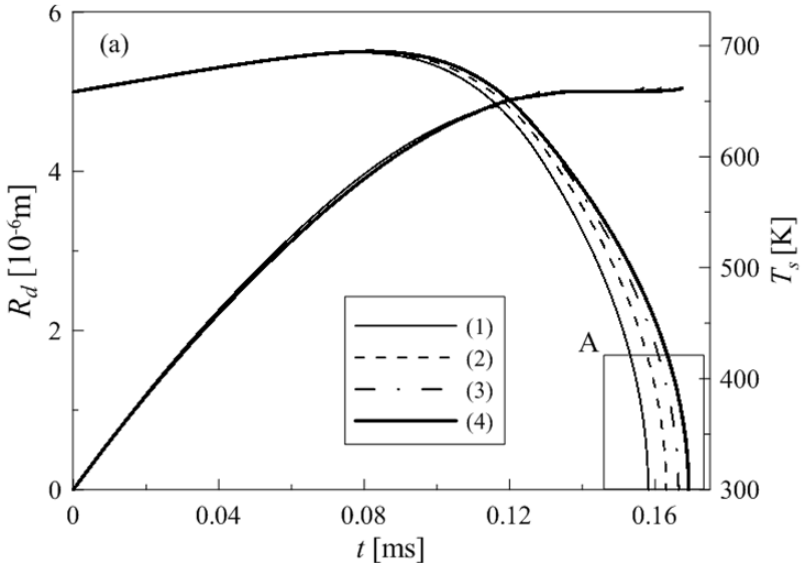
# **Application**: heating and evaporation of fuel droplet

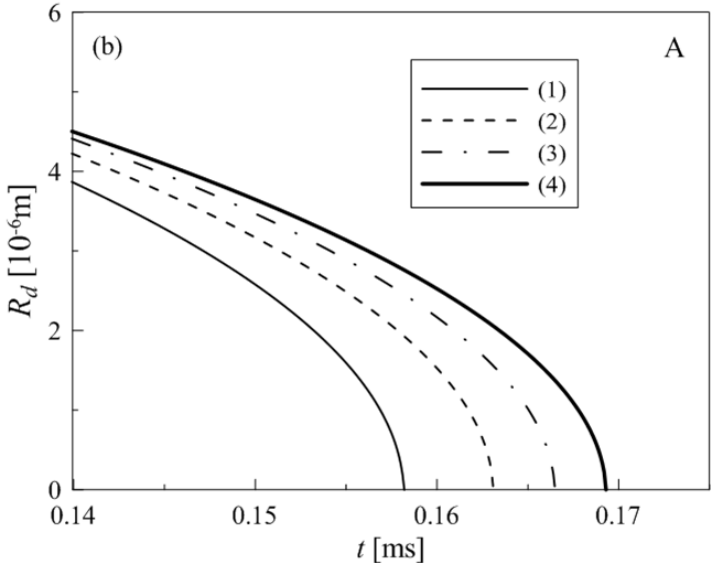



Initial parameters:

$P_0$ = 30 bar
$T_{g0}$ = 1,500 K
$T_s$ = 300 K
$R_0$ = 5 μm

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



# Summary

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

  → **Kinetic Boundary Condition**
- Kinetic modelling of evaporation in kinetic region, taking into account the inelastic collision
- Application to engines: heating and evaporation of Diesel fuel droplet in engine-like conditions and longer evaporation time prediceted
- Other applications: evaporation/condensation of other fuel molecules, micro-electro-mechanical system (MEMS) and nano-electro-mechanical system (NEMS)

# Publications


- Sazhin, S.S, Xie, J.-F, Shishkova, I.N, Elwardany, A.E and Heikal, M.R (2012). ``A kinetic model of droplet heating and evaporation: effects of inelastic collisions and non-unity evaporation coefficient'', **International Journal of Mass and Heat Transfer** (in press).
- Shishkova, I.N, Sazhin, S.S and Xie, J.-F (2012). ``A solution of the Boltzmann equation in the presence of inelastic collisions'', **Journal of Computational Physics** (in press).
- Xie, J.-F, Sazhin, S.S and Cao, B.-Y (2012). ``Molecular dynamics study of condensation/evaporation and velocity distribution of n-dodecane at liquid-vapour phase equilibria'', **Journal of Thermal Science and Technology** 7, 288-300.
- Xie, J.-F, Sazhin, S.S and Cao, B.-Y (2011). ``Molecular dynamics study of the processes in the vicinity of the n-dodecane vapour/liquid interface'', **Physics of Fluids** 23, 112104.
- Cao, B.-Y, Xie, J.-F and Sazhin, S.S (2011). ``Molecular dynamics simulation on evaporation and condensation of n-dodecane at liquid-vapour phase equilibria'', **Journal of Chemical Physics** 134, 164309.

# THANK YOU