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MODELLING OF AUTOMOTIVE FUEL DROPLET HEATING AND EVAPORATION

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Concept

(Engineering Mathematics)

Modelling of individual processes (numerical or analytical)

Example: modelling of deformation of individual droplets

Strength: allows in-depth analysis and understanding of underlying physics

Weakness: does not take into account the effects of other processes in realistic engineering systems

Concept

(Computational Fluid Dynamics)

Modelling of realistic engineering systems (numerical)

Example: modelling of Diesel engines

Strength: takes into account the interaction between various processes (fluid dynamics, heat/mass transfer etc)

Weakness: too simplistic models for individual processes are used; difficult to understand the underlying physics

Analysis of realistic engineering systems requires a combined approach using the methods of engineering mathematics and Computational Fluid Dynamics (CFD)

MODELS FOR DOPLET HEATING AND EVAPORATION (*Conventional CFD models*)

1. The Infinite Thermal Conductivity (ITC) models based on the energy balance equation of the droplet as a whole were used.

2. Droplets were assumed to be opaque grey spheres.

3. Droplet radii were assumed to be constant during each time step.

4. Too complex or too simplistic models for heating and evaporation of multi-component droplets were used.

5. Kinetic and molecular dynamic effects on droplet evaporation were ignored

Conduction limit. Effective conductivity

$$c_1\rho_1\frac{\partial T}{\partial t} = k_1\left(\frac{\partial^2 T}{\partial R^2} + \frac{2}{R}\frac{\partial T}{\partial R}\right) + P\,(R)$$

$$h(T_g - T_s) = -\rho_1 L\dot{R}_d + k_1\left.\frac{\partial T}{\partial R}\right|_{R=R_d}$$

$$k_{\text{eff}} = \chi_T k_l,$$

where the coefficient χ_T varies from about 1 (at droplet Peclet number $\text{Pe}_{d(l)} = \text{Re}_{d(l)}\text{Pr}_l < 10$) to 2.72 (at $\text{Pe}_{d(l)} > 500$) and can be approximated as

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

$$P(R)\big|_{R<R_d} = 3\times10^6 \quad a \quad \sigma \quad R_d^b\,\theta_R^4 \big/ c_l\rho_l$$

$$P(R)\big|_{R>R_d} = 0$$

where ϑ_R is the radiation temperature, R_d is the droplet radius,

$$a = \mathrm{a}_0 + \mathrm{a}_1\theta_\mathrm{R}/10^3 + \mathrm{a}_2(\theta_\mathrm{R}/10^3)^2,$$

$$b = \mathrm{b}_0 + \mathrm{b}_1\theta_\mathrm{R}/10^3 + \mathrm{b}_2(\theta_\mathrm{R}/10^3)^2,$$

ϑ_R can be assumed equal to the external temperature T_{ext} in the case of an optically thin gas in the whole domain.

Analytical solution for *h*=const

$$T(r,t)=\frac{1}{r}\sum_{n=1}^{\infty}\left\{\frac{p_n}{\kappa\lambda_n^2}+\exp\left[-\kappa\lambda_n^2 t\right]\left(q_n-\frac{p_n}{\kappa\lambda_n^2}\right)-\frac{\sin\lambda_n}{\|\,v_n\,\|^2\,\lambda_n^2}\mu_0(0)\right.$$

$$\left.\times\exp\left[-\kappa\lambda_n^2 t\right]-\frac{\sin\lambda_n}{\|\,v_n\,\|^2\,\lambda_n^2}\int_0^t\frac{\mathrm{d}\mu_0(\tau)}{\mathrm{d}\tau}\exp\left[-\kappa\lambda_n^2(t-\tau)\right]\mathrm{d}\tau\right\}\sin\lambda_n r+T_{\mathrm{eff}}(t),$$

where λ_n are positive solutions (in ascending order) of the equation:

$\lambda\cos\lambda+h_0\sin\lambda=0$, $h_0=(hR_d/k_l)-1=\mathrm{const}$, $r=R/R_d$, $\kappa=\frac{k_l}{c_l\rho_l R_d^2}$,

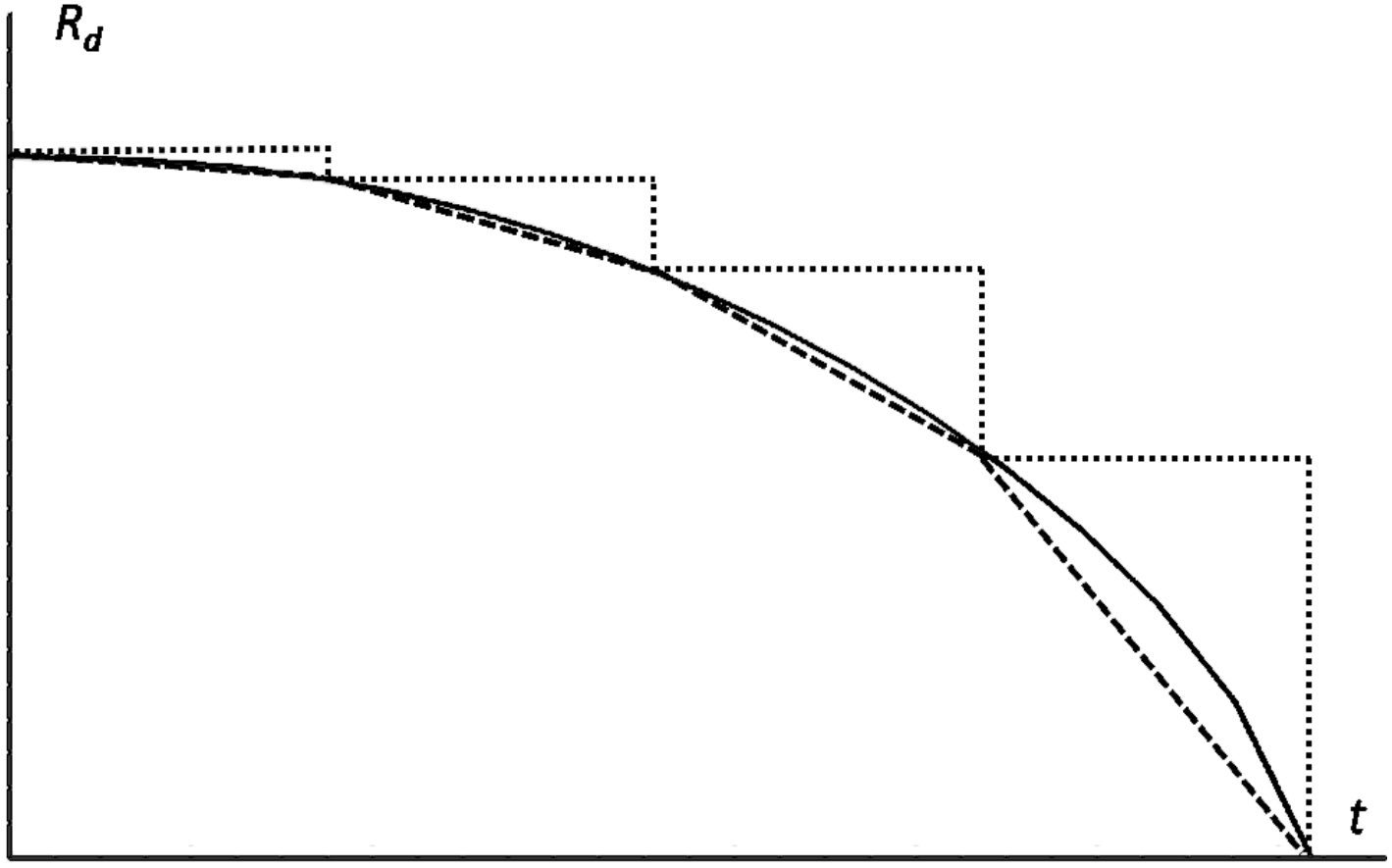
$$T_{\mathrm{eff}}=T_g+\frac{\rho_l L\dot{R}_d}{h},\qquad \mu_0(t)=\frac{hT_{\mathrm{eff}}(t)R_d}{k_l},$$

$$\|\,v_n\,\|^2=\frac{1}{2}\left(1-\frac{\sin 2\lambda_n}{2\lambda_n}\right)=\frac{1}{2}\left(1+\frac{h_0}{h_0^2+\lambda_n^2}\right\},$$

$$q_n=\frac{1}{\|\,v_n\,\|^2}\int_0^1\tilde{T}_0(r)v_n(r)\mathrm{d}r,\qquad \tilde{T}_0(r)=rT_0(rR_d).$$

$$p_n=\frac{1}{\|\,v_n\,\|^2}\int_0^1\tilde{P}(r)v_n(r)\mathrm{d}r,\qquad \tilde{P}(r)=rP(r),\qquad r=R/R_d$$

Effect of the moving interface



Effect of the moving interface

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

for $0 \leq t \leq t_e$, $0 \leq R \leq R_d(t)$, where κ is liquid thermal diffusivity ($\kappa = k_l/(c_l \rho_l)$ =const), k_l is the liquid thermal conductivity, c_l is the liquid specific heat capacity, ρ_l is the liquid density, R is the distance from the centre of the droplet.

$$\left(k_l \frac{\partial T}{\partial R} + hT \right) \Big|_{R=R_d(t)} = hT_g + \rho_l L \dot{R}_d(t)$$

$$T(t=0) = T_0(R)$$

$$\dot{R}_d = -\frac{k_g \ln(1+B_M)}{\rho_l c_{pg} R_d}$$

$$R_d(t) = R_{d0}(1+\alpha t)$$

Analytical solution

$$T(R) = \frac{1}{R\sqrt{R_d(t)}} \exp\left[-\frac{\alpha R_{d0} R^2}{4\kappa R_d(t)}\right] \left[\sum_{n=1}^{\infty} \Theta_n(t) \sin\left(\lambda_n \frac{R}{R_d(t)}\right) + \frac{\mu_0(t)}{1+h_0} \frac{R}{R_d(t)}\right]$$

$$\Theta_n(t) = q_n \exp\left[-\frac{\kappa \lambda_n^2 t}{R_{d0} R_d(t)}\right] + f_n \mu_0(t)$$

$$-f_n \kappa \lambda_n^2 \int_0^t \frac{\mu_0(\tau)}{R_d^2(\tau)} \exp\left[\frac{\kappa \lambda_n^2}{\alpha R_{d0}} \left(\frac{1}{R_d(t)} - \frac{1}{R_d(\tau)}\right)\right] \mathrm{d}\tau.$$

$$f_n = \frac{1}{|| \, v_n \, ||^2} \int_0^1 f(\xi) v_n(\xi) \mathrm{d}\xi = -\frac{\sin \lambda_n}{|| \, v_n \, ||^2 \, \lambda_n^2}$$

$$\lambda \cos \lambda + h_0 \sin \lambda = 0$$

$$|| \, v_n \, ||^2 = \frac{1}{2}\left(1 - \frac{\sin 2\lambda_n}{2\lambda_n}\right) = \frac{1}{2}\left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right)$$

$$h_0 = \frac{h(t)}{k_l} R_d(t) - 1 - \frac{R_d'(t) R_d(t)}{2\kappa}$$

Sazhin, S.S., Krutitskii, P.A., Gusev, I.G., Heikal, M. (2010) Transient heating of an evaporating droplet, Int. J Heat Mass Transfer, **53** (13-14), 2826-2836

Discrete Components Model

$$k_{\text{eff}} = \chi k_l$$

$$\frac{\partial Y_{li}}{\partial t} = D_l \left(\frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right)$$

$$\alpha(\epsilon_i - Y_{lis}) = -D_l \left. \frac{\partial Y_{li}}{\partial R} \right|_{R=R_d-0}$$

$$\alpha = \frac{|\dot{m}_d|}{4\pi\rho_l R_d^2}$$

$$D_{\text{eff}} = \chi_Y D_l$$

$$p_{vi} = X_{li}\gamma_i p_{vi}^*$$

Solution to the species diffusion equation

$$Y_{li} = \epsilon_i + \frac{1}{R}\left\{\exp\left[D_l\left(\frac{\lambda_0}{R_d}\right)^2 t\right][q_{i0} - \epsilon_i(0)Q_0]\sinh\left(\lambda_0\frac{R}{R_d}\right)\right.$$

$$\left. + \sum_{n=1}^{\infty}\exp\left[-D_l\left(\frac{\lambda_n}{R_d}\right)^2 t\right][q_{in} - \epsilon(0)Q_n]\sin\left(\lambda_n\frac{R}{R_d}\right)\right\}.$$

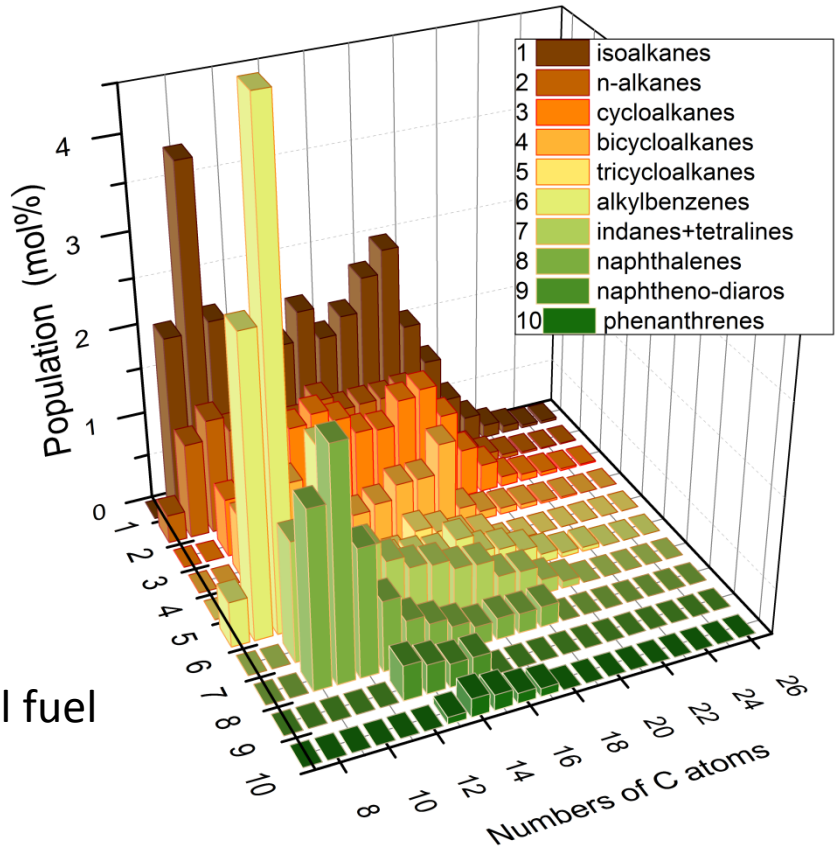
$$\tanh\lambda = -\frac{\lambda}{h_0}$$

$$\tan\lambda = -\frac{\lambda}{h_0}.$$

$$v_0(R) = \sinh\left(\lambda_0\frac{R}{R_d}\right)$$

$$v_n(R) = \sin\left(\lambda_n\frac{R}{R_d}\right)$$

Multi-Dimensional Quasi-Discrete Model

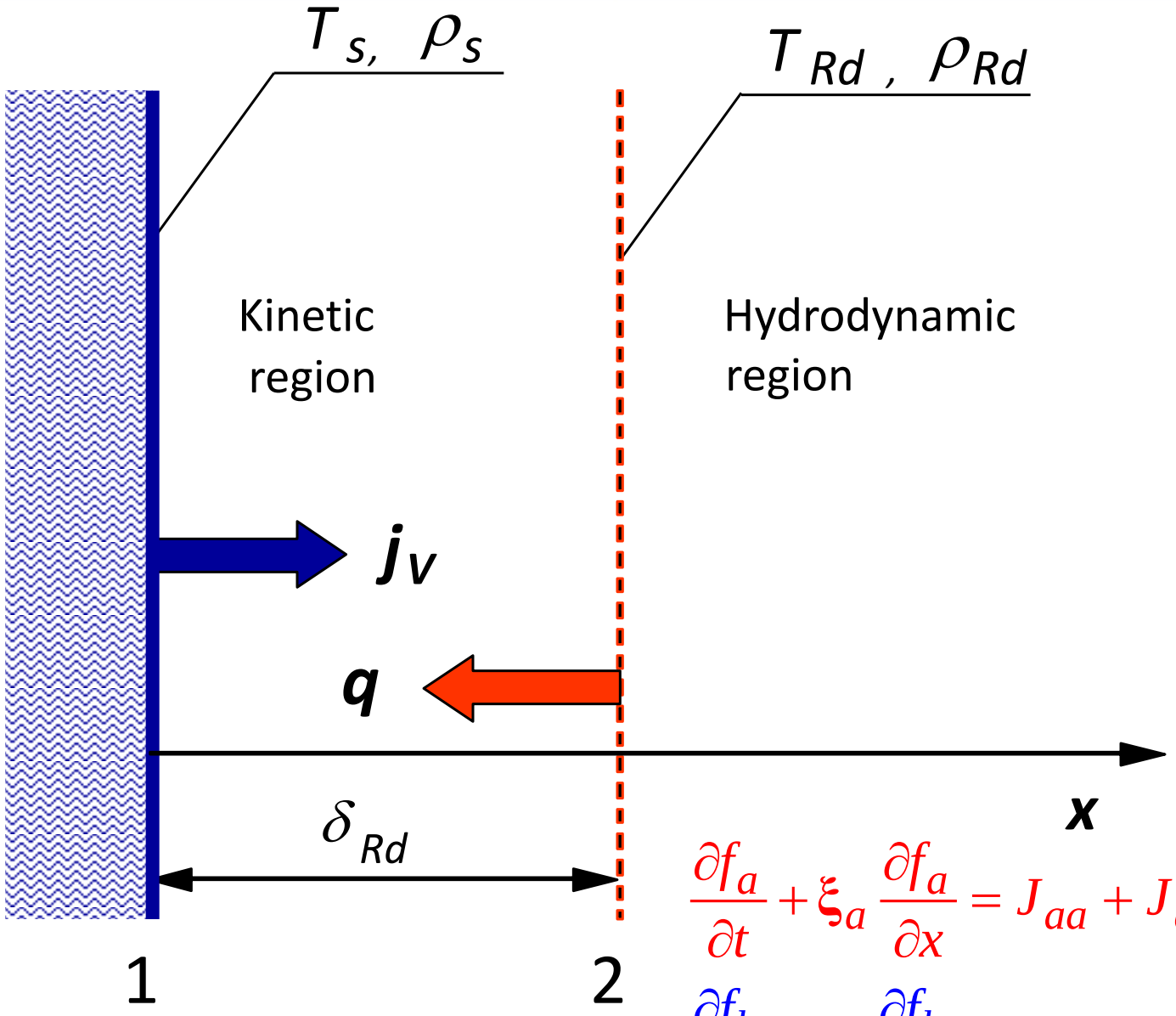


Realistic Diesel fuel

Multi-Dimensional Quasi-Discrete Model

m	Component
1	alkanes
2	cycloalkanes
3	bicycloalkanes
4	alkylbenzenes
5	indanes & tetralines
6	naphthalenes
7	tricycloalkane
8	diaromatic
9	phenanthrene

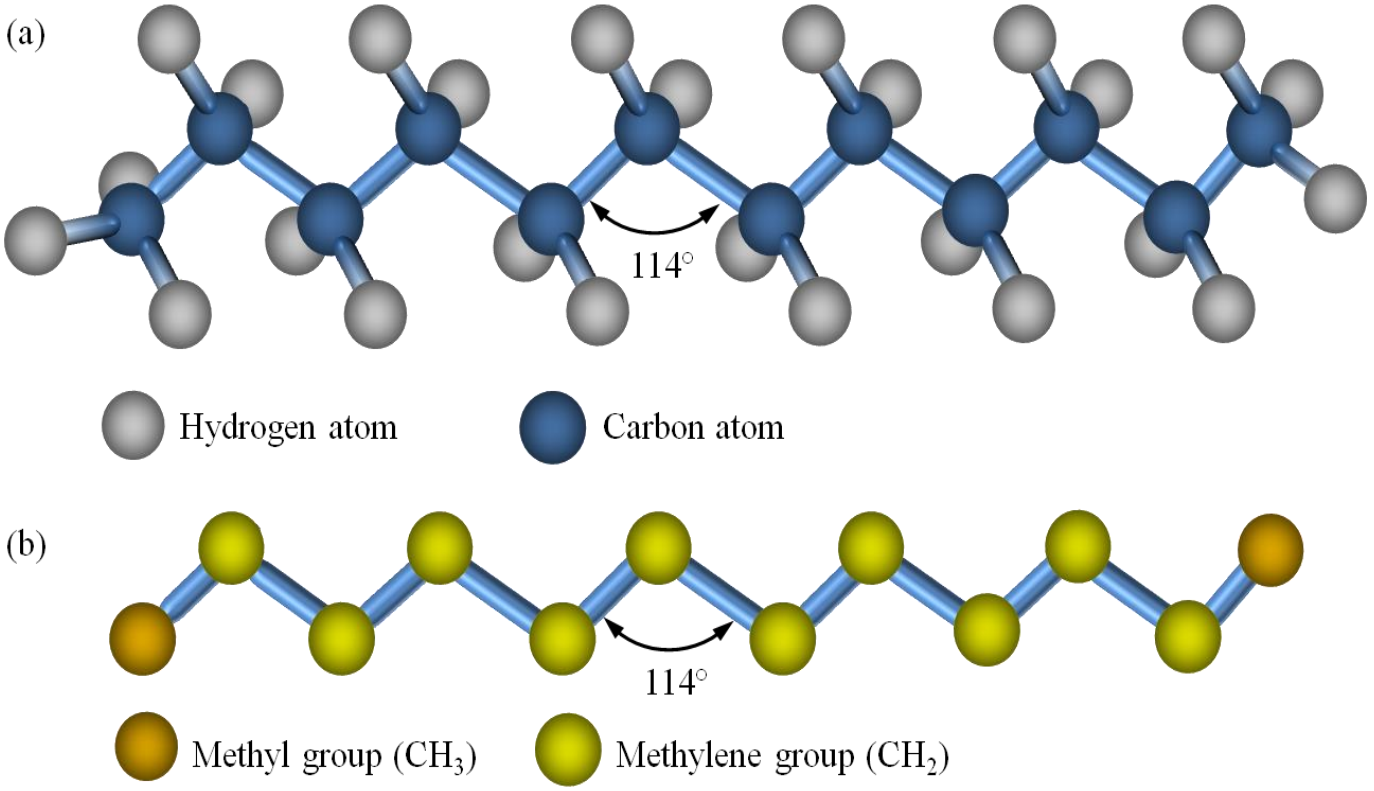
$$
\left.
\begin{aligned}
\overline{n}_{1m} &= \frac{\sum_{n=n_{1m}}^{n=n_{(\varphi_m+1)m}} (nX_{nm})}{\sum_{n=n_{1m}}^{n=n_{(\varphi_m+1)m}} X_{nm}}, \\
\overline{n}_{2m} &= \frac{\sum_{n=n_{(\varphi_m+2)m}}^{n=n_{(2\varphi_m+2)m}} (nX_{nm})}{\sum_{n=n_{(\varphi_m+2)m}}^{n=n_{(2\varphi_m+2)m}} X_{nm}}, \\
\overline{n}_{3m} &= \frac{\sum_{n=n_{(2\varphi_m+3)m}}^{n=n_{(3\varphi_m+3)m}} (nX_{nm})}{\sum_{n=n_{(2\varphi_m+3)m}}^{n=n_{(3\varphi_m+3)m}} X_{nm}}, \\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
\overline{n}_{\ell m} &= \frac{\sum_{n=n_{((\ell-1)\varphi_m+\ell)m}}^{n=n_{k_m}} (nX_{nm})}{\sum_{n=n_{((\ell-1)\varphi_m+\ell)m}}^{n=n_{k_m}} X_{nm}},
\end{aligned}
\right\}
$$



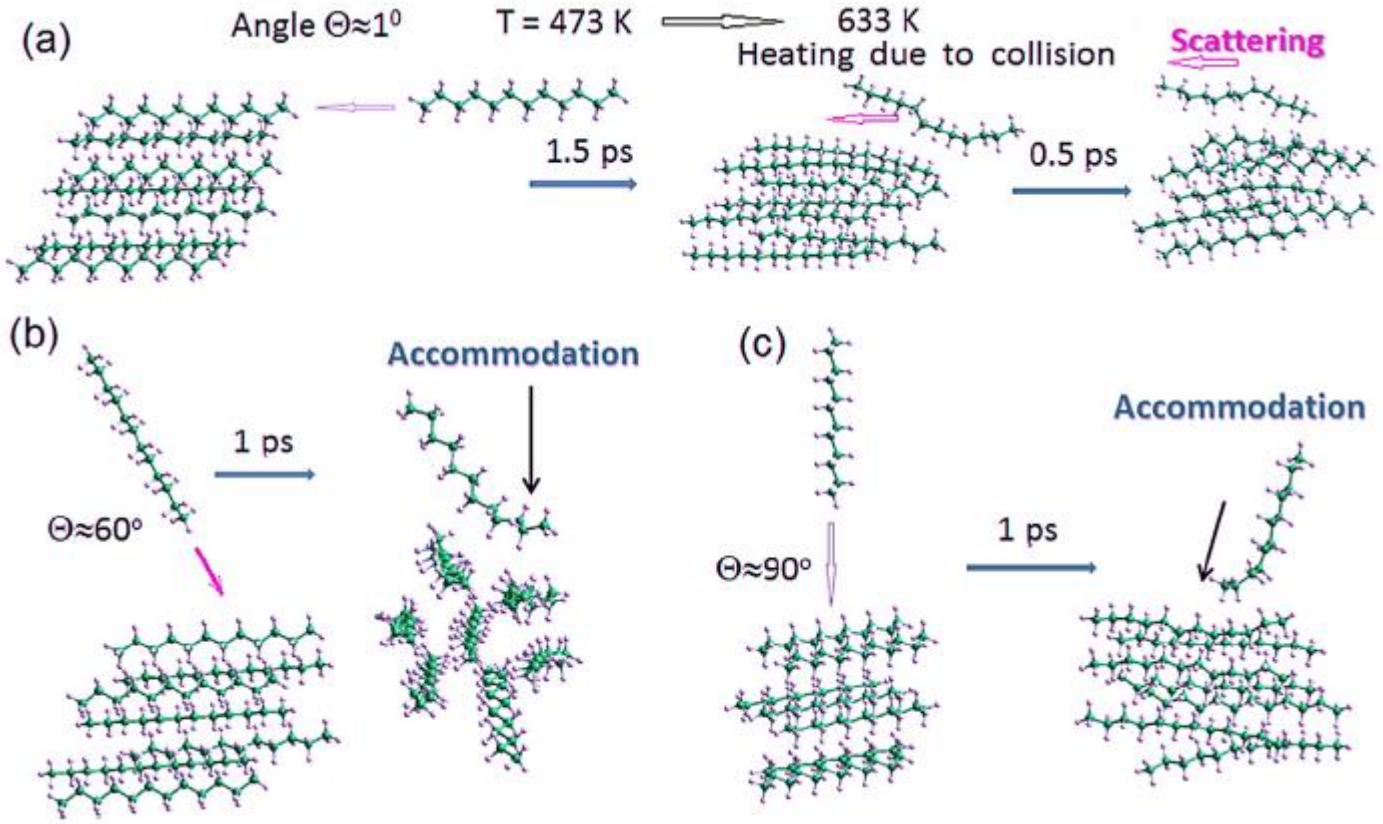
$$\frac{\partial f_a}{\partial t} + \xi_a \frac{\partial f_a}{\partial x} = J_{aa} + J_{ab},$$

$$\frac{\partial f_b}{\partial t} + \xi_b \frac{\partial f_b}{\partial x} = J_{ba} + J_{bb},$$

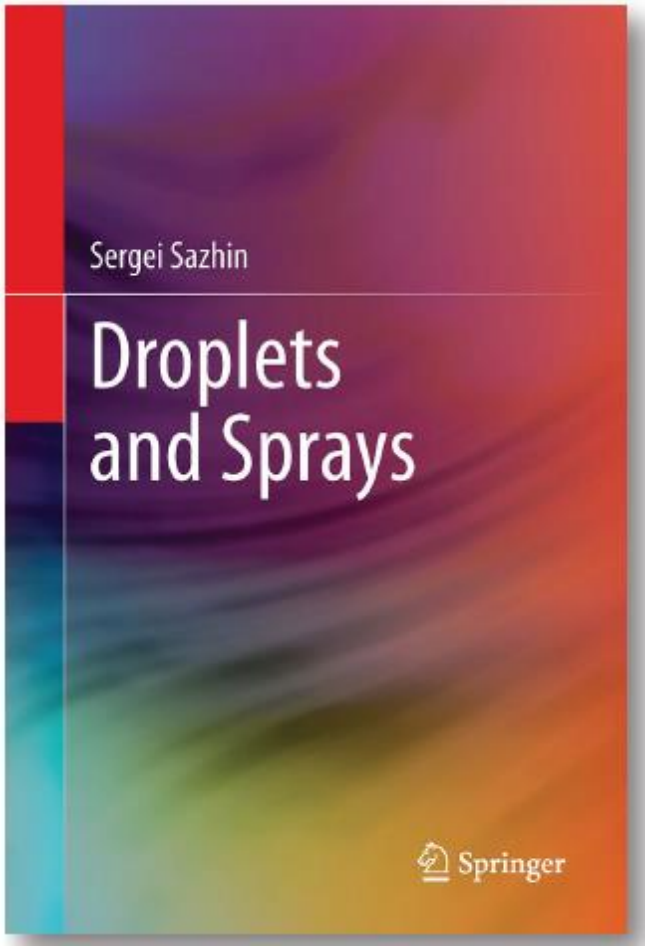
United Atom Model (UAM)



A study of the evaporation and condensation of n-alkane clusters and nanodroplets using quantum chemical methods



Gun'ko, V.M., Nasiri, R., Sazhin, S.S. (2014) A study of the evaporation and condensation of n-alkane clusters and nanodroplets using quantum chemical methods, *Fluid Phase Equilibria*, **366** 99-107.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Droplets and Sprays
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