A quasi-discrete model for droplet heating and evaporation: application to Diesel and gasoline fuels

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Research workshop: Droplets and Sprays: modelling and experimentation

13th January 2012

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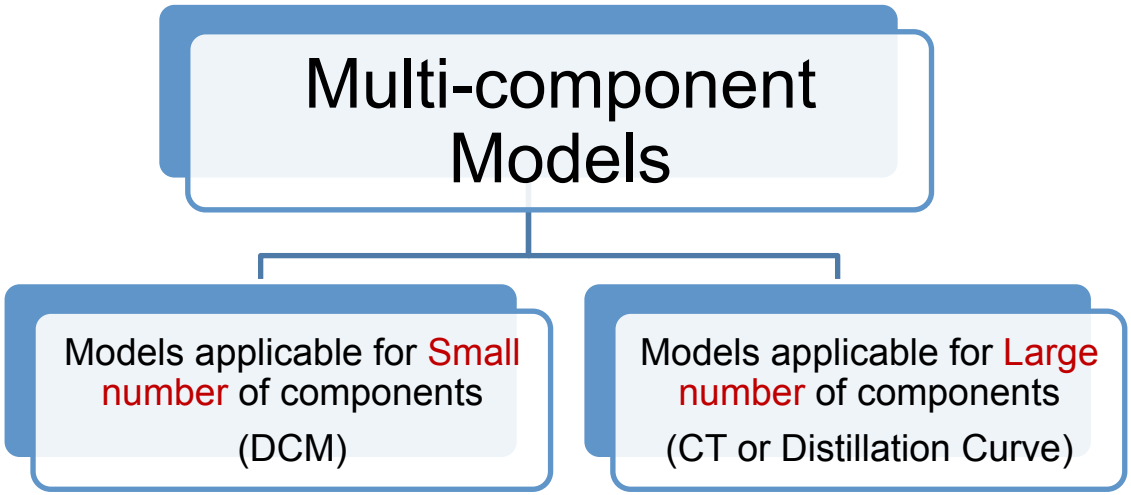
Plan

- Introduction
- Concept of quasi-component
- Thermophysical properties of n-alkanes
- Preliminary results for Diesel fuel
- Advanced results for Diesel and gasoline fuels
- Conclusions

Introduction

- Models for multi-component droplets can be subdivided into two groups:



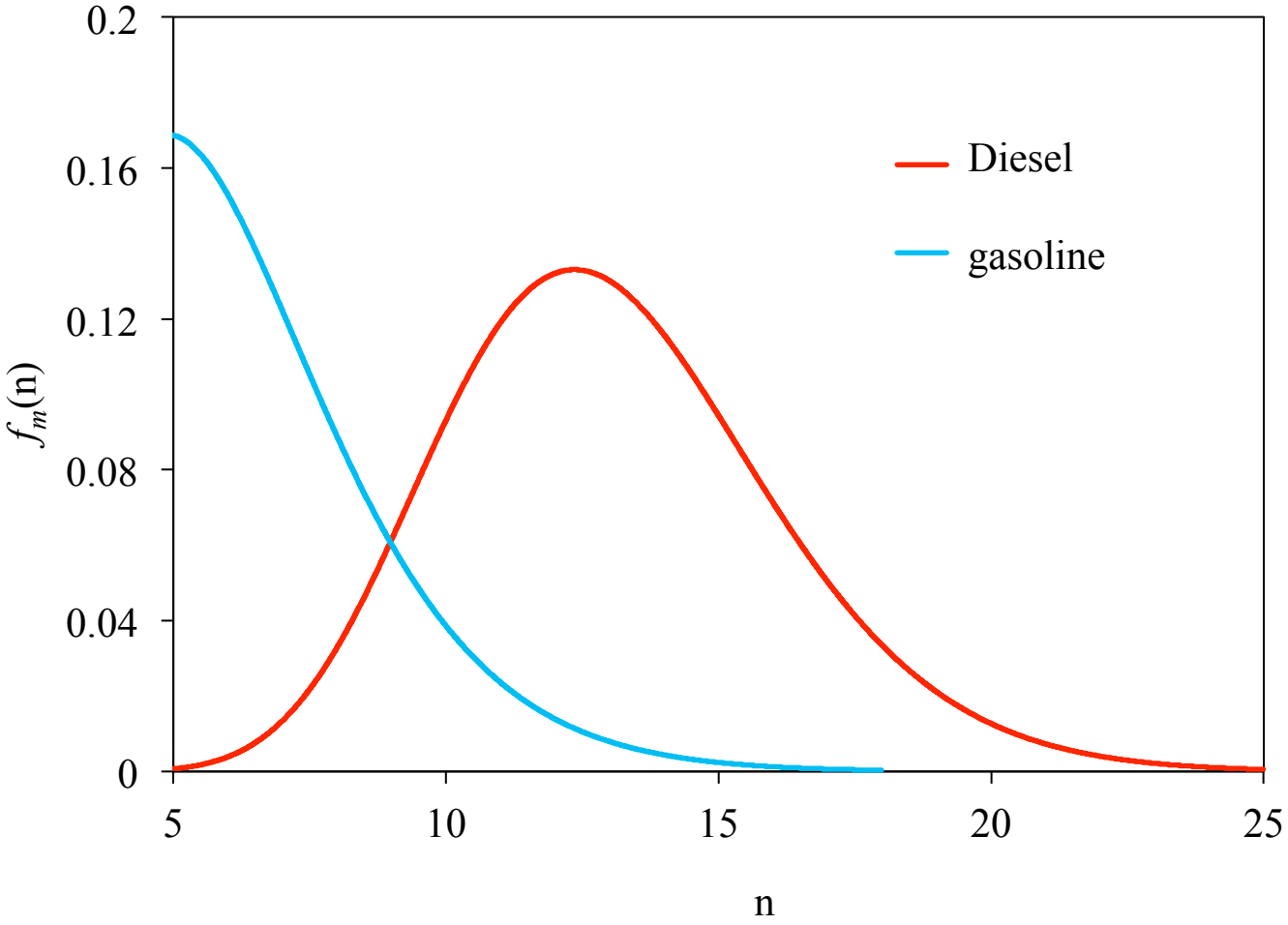
- Most of these models assume that the species diffusivity within the droplet is assumed to be infinitely large or small while each component has its own volatility.

Concept of quasi-discrete model

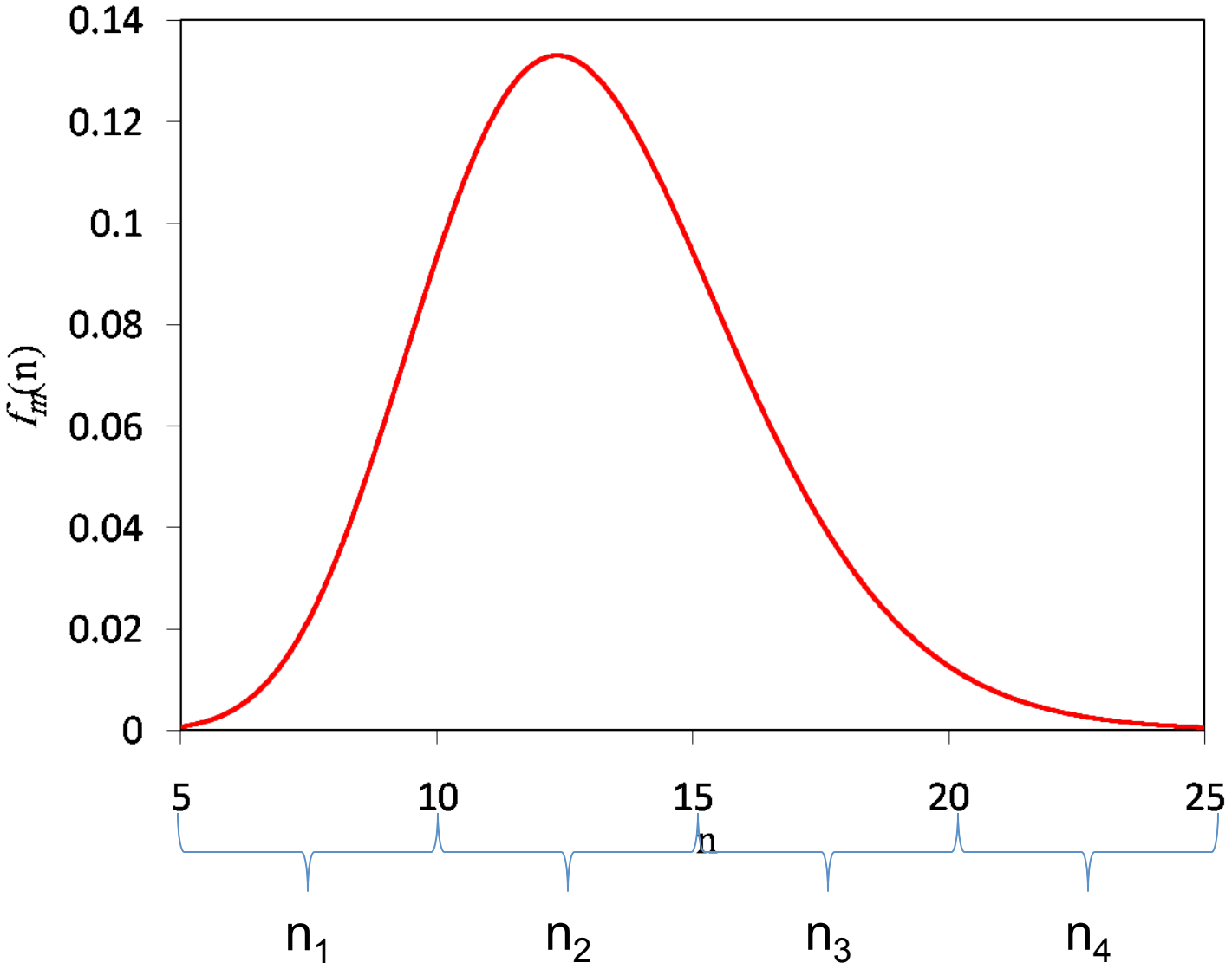
Concept of quasi-discrete model

- The model is based on the assumption that the components can be described as C_nH_{2n+2} (n-alkanes).
- The model is based on replacing a large number of actual components with a small number of quasi-components.
- These quasi-components are then treated as actual components, taking into account the diffusion of quasi-components in droplets.

Concept of quasi-discrete model



Concept of quasi-discrete model



Concept of quasi-discrete model

- The initial mole fraction of each quasi-component is calculated as:

$$X_j = \int_{n_{j-1}}^{n_j} f_m(n)\mathrm{d}n$$

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

- where $M(n) = 14n + 2$ are the molecular weights, $n_0 = 5$, $n_f = 25$, $\Gamma(\alpha)$ is Gamma function, and α, β, γ are parameters that determine the shape of the distribution and the original shift.

Concept of quasi-discrete model

- Following Arias-Zugasti and Rosner (2003), we assumed that: $\alpha = 18.5$,$\beta = 10$ and $\gamma = 0$ (Diesel Fuel)

  $\alpha = 5.7, \beta = 15$ and $\gamma = 0$ (gasoline fuel)

- The choice of $C_m(n_0, n_f)$ assures that:

$$\int_{n_0}^{n_f} f_m(n)\mathrm{d}n = 1$$

- Each quasi-component carbon atoms estimated as:

$$\bar{n}_j = \frac{\int_{n_{j-1}}^{n_j} n f_m(n)\mathrm{d}n}{\int_{n_{j-1}}^{n_j} f_m(n)\mathrm{d}n}$$

Thermophysical properties of n-alkanes

- Critical and Boiling Temperatures

Following Poling et al (2000), the dependence of critical and boiling temperatures on number of carbon atoms *n*:

$$T_{cr}(n) = a_{cr} + b_{cr}n + c_{cr}n^2 + d_{cr}n^3$$

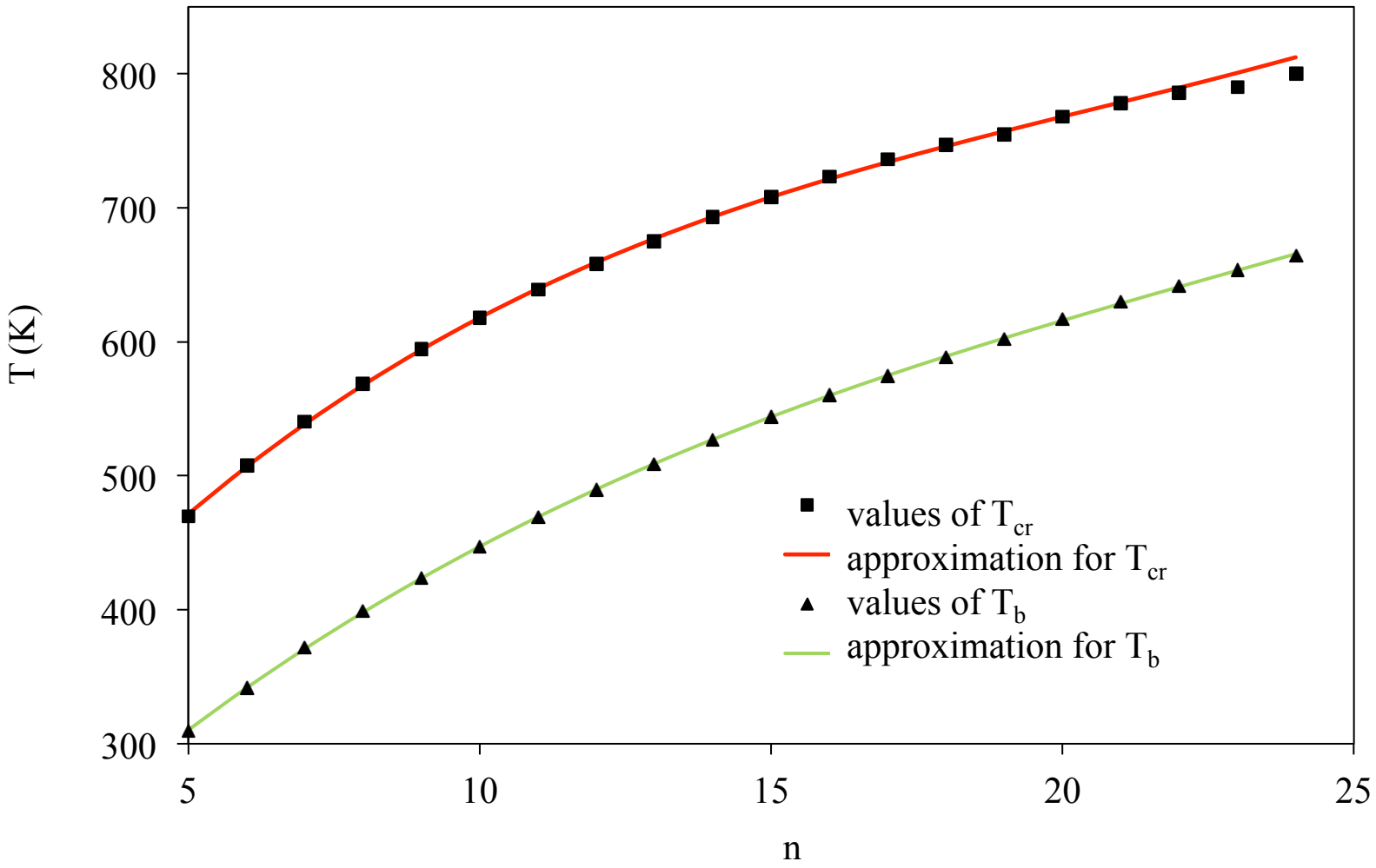
$$T_b(n) = a_b + b_b n + c_b n^2 + d_b n^3$$

where the constants are:

Coefficient	*a*	*b*	*c*	*d*
Critical	242.3059898052	55.9186659144	- 2.1883720897	0.0353374481
Boiling	118.3723701848	44.9138126355	- 1.4047483216	0.0201382787

Poling B.E., Prausnitz J.M. and O'Connell J., (2000), *The Properties of Gases and Liquids,* New York: McGraw-Hill.

- Critical and Boiling Temperatures



- Saturation pressure and Latent heat of vaporization

Following Arias-Zugasti and Rosner (2003) the saturation pressure of n-alkanes (*n* = 4-17).

$$p_{sat}(n) = \exp\left(A(n) - \frac{B(n)}{T_s - C(n)}\right)$$

where $A(n) = 6.318n^{0.05091}$, $B(n) = 1178n^{0.4652}$ and $C(n) = 9.467n^{0.9143}$

Latent heat:

$$L(n) = \frac{R_u B(n) T_s^2}{M(n)(T_s - C(n))^2}$$

where $M(n) = 14n + 2$

Arias-Zugasti M, Rosner DE. *Multicomponent fuel droplet vaporization and combustion using spectral theory for a continuous mixture*. Combustion and Flame 2003;135:271-284.

- Liquid Density

Following Yaws (2008), the dependence of liquid density on number of carbon atoms *n* and temperature (*n* = 5-25):

$$\rho_l(n,T) = 1000 \times A_\rho(n) \times B_\rho(n)^{-\left(1-\frac{T}{T_{cr}(n)}\right)^{C_\rho(n)}}$$

The values of $A(n)$, $B(n)$ and $C(n)$ are approximated as follows:

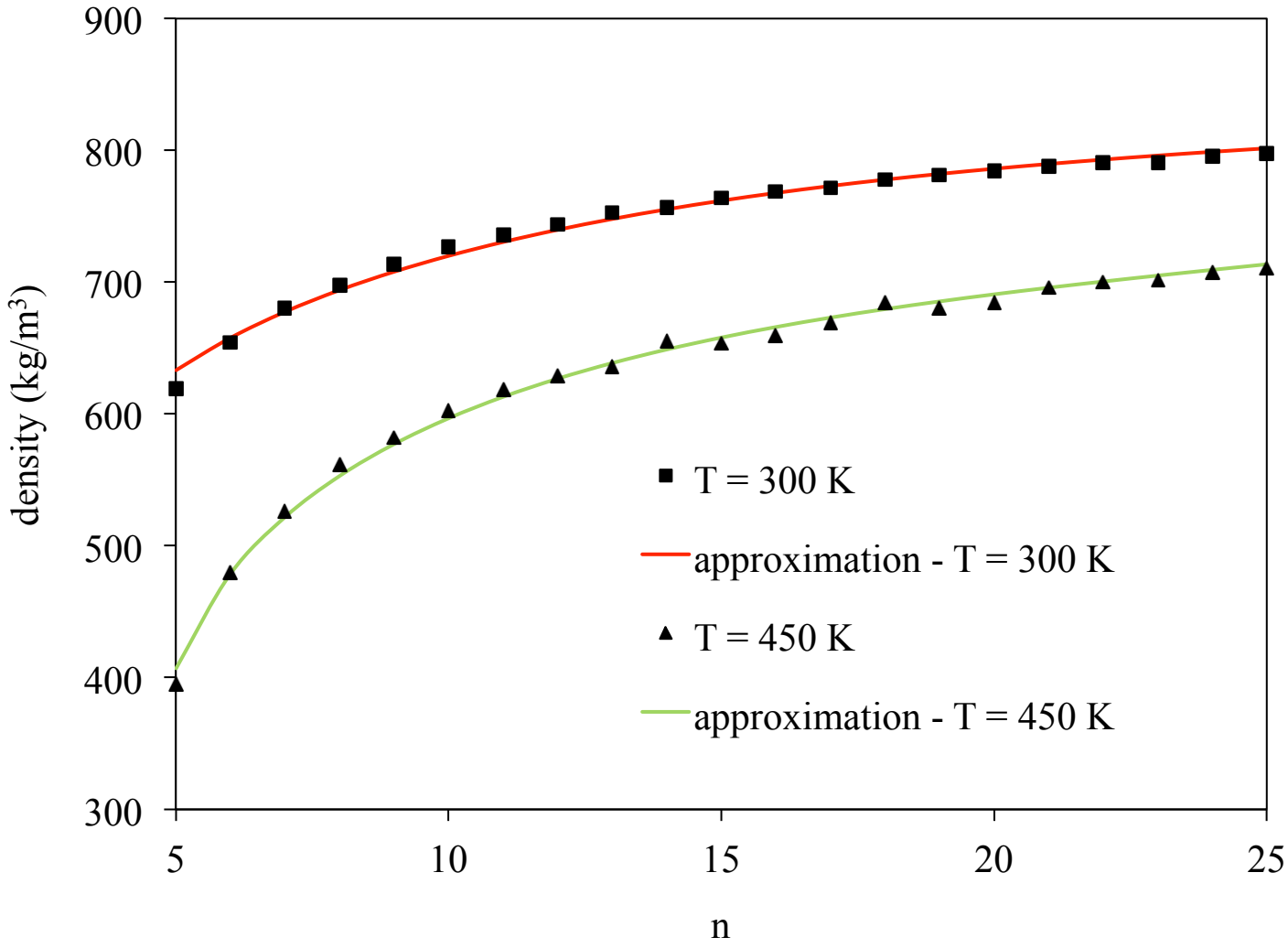
$$A_\rho(n) = 0.00006196104 \times n + 0.234362$$

$$B_\rho(n) = 0.00004715697 \times n^2 - 0.00237693 \times n + 0.2768741$$

$$C_\rho(n) = 0.000597039 \times n + 0.2816916$$

Yaws C.L., (2008), *Thermophysical properties of chemicals and hydrocarbons*, William Andrew.

- Liquid Density



- Liquid Viscosity

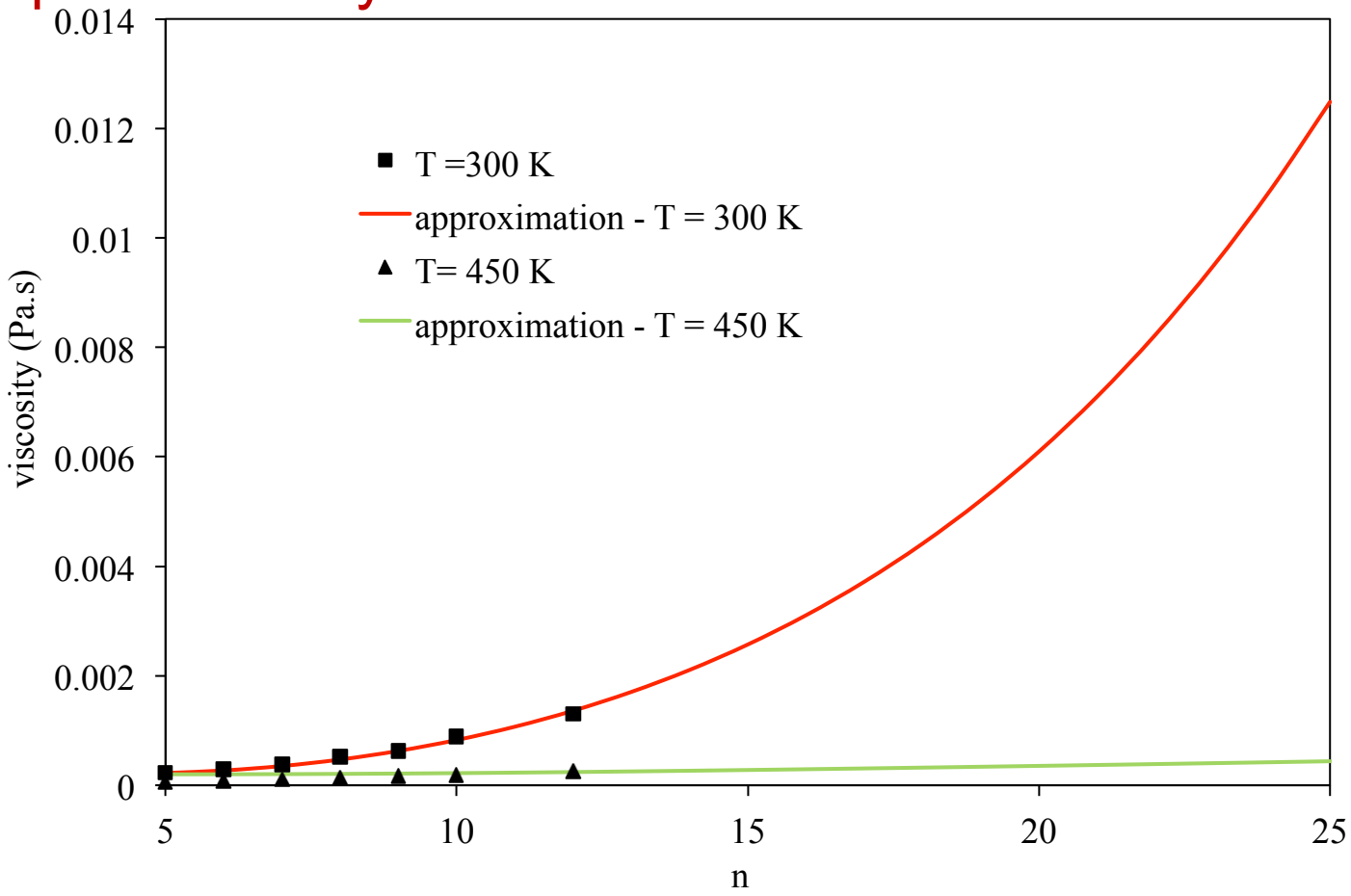
Following Mehrotra (1994), the dependence of liquid viscosity on number of carbon atoms *n* and temperature (*n* = 4-44):

$$\mu_l(n,T) = 10^{-3}\left(10^{\left[100(0.01T)^{b(n)}\right]} - 0.8\right)$$

where $b(n) = -5.745 + 0.616\ln(n) - 40.468n^{-1.5}$

Mehrotra A.K. (1994), *Correlation and prediction of the viscosity of pure hydrocarbon*, The Canadian Journal of Chemical Engineering, (72) 554-557.

- Liquid Viscosity



The approximations are reproduced using the equation suggested by Mehrotra (1994). The symbols are reproduced from http://webbook.nist.gov/chemistry/

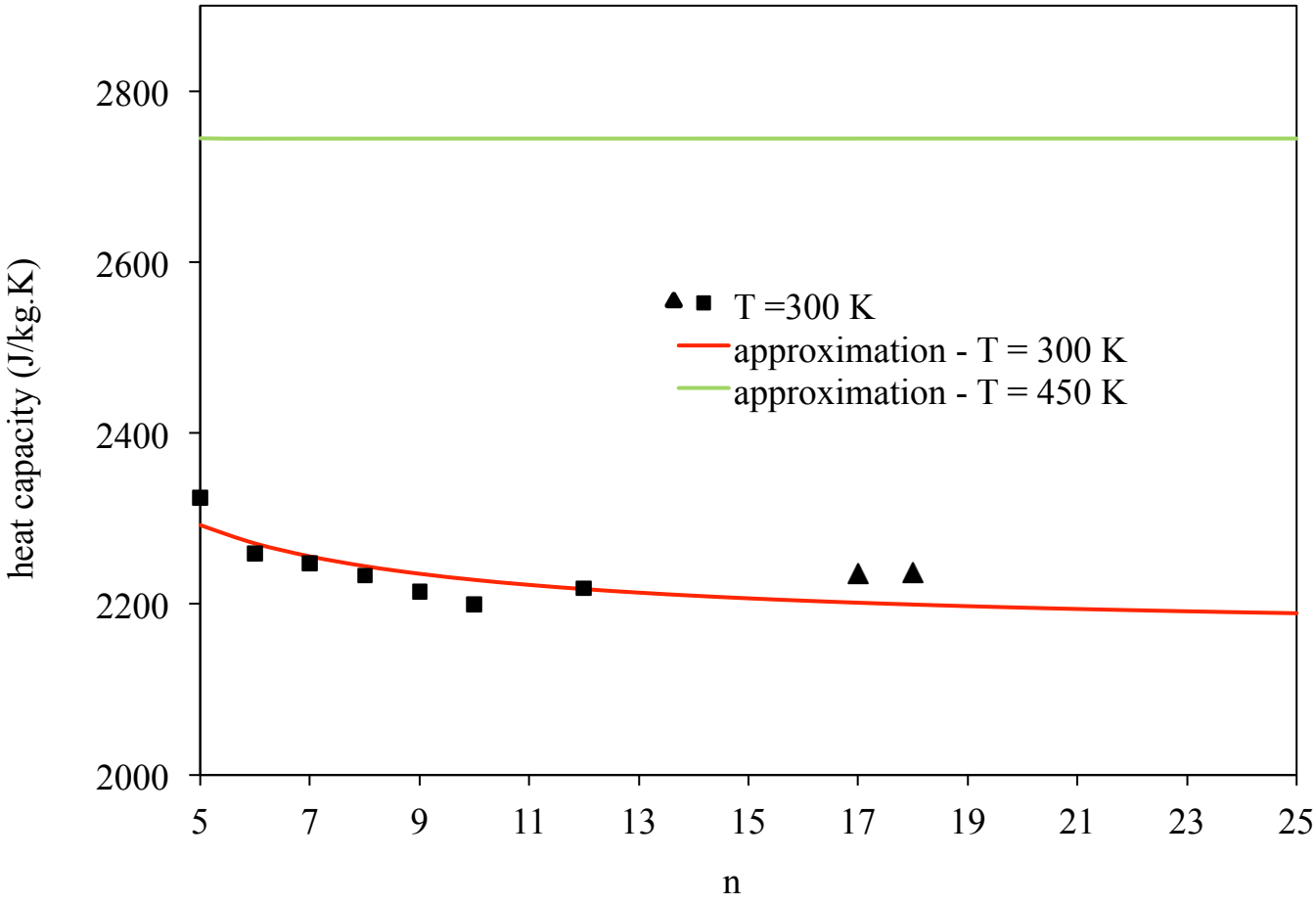
- Liquid Heat Capacity

Following van Miltenburg (2000), the dependence of liquid heat capacity on number of carbon atoms *n* and temperature (*n* = 2-26):

$$c_{p,l}(n,T) = 1000\left(\frac{43.9 + 13.99(n-1) + 0.0543(n-1)T}{M(n)}\right)$$

van Miltenburg J.C.(2000), Fitting the heat capacity of liquid n-alkanes: new measurements of n-heptadecane and n-octadecane, Thermochimica Acta (343) 57-62.

- Liquid Heat Capacity



The data of *n-heptadecane and n-octadecane* (triangles) reproduced from van Miltenburg (2000), the other data (squares) reproduced from http://webbook.nist.gov/chemistry/.

- Liquid Thermal Conductivity

Following Yaws (1995), the dependence of liquid thermal conductivity on number of carbon atoms *n* and temperature (*n* = 5-20):

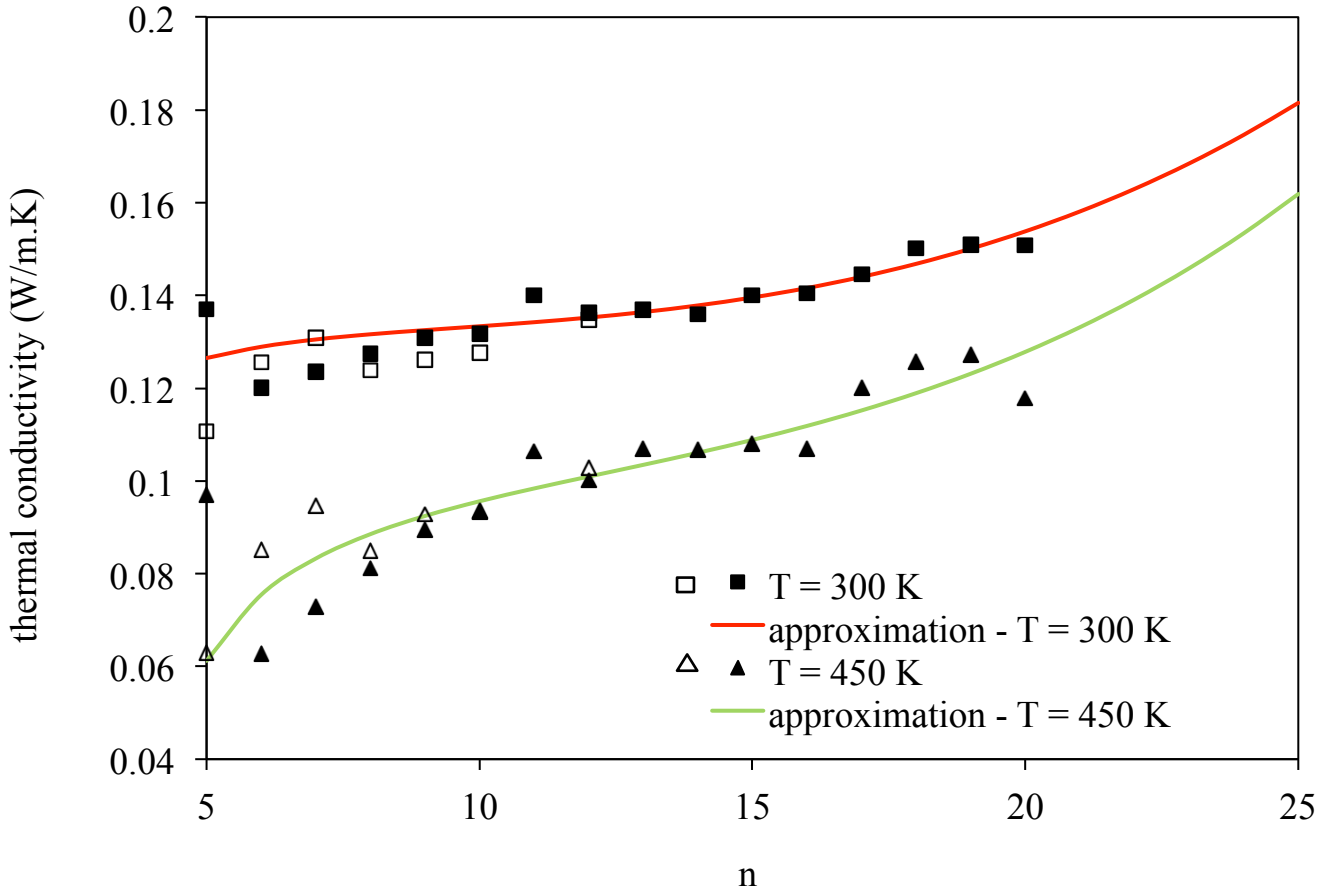
$$k_l(n,T) = 10^{\left[A_k(n)+B_k(n)\left(1-\frac{T}{T_{cr}(n)}\right)^{2/7}\right]}$$

where $A_k(n) = 0.002911 \times n^2 - 0.071339 \times n - 1.319595$

$$B_k(n) = -0.002498 \times n^2 + 0.058720 \times n + 0.710698$$

Yaws C.L., (1995), *Handbook of thermal conductivity,* Vol (2): Organic compounds, C_5 to C_7 and Vol (3): Organic compounds, C_8 to C_{28}. Gulf Publishing Company, Houston, Texas, USA.

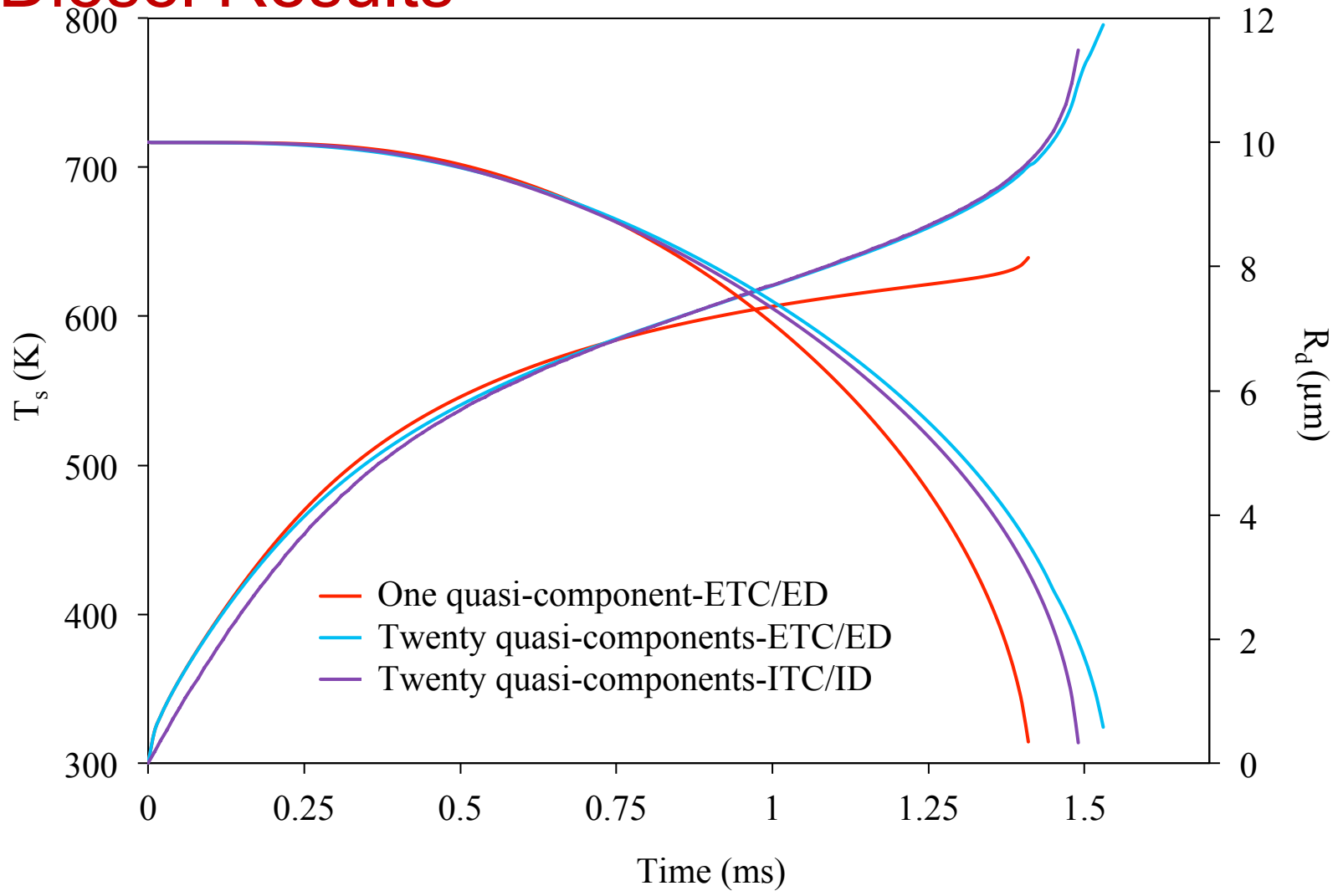
- Liquid Thermal Conductivity



Hollow symbols are reproduced from http://webbook.nist.gov/chemistry/.
Solid Symbols are reproduced form Yaws (1995) using the corresponding values of the constants.

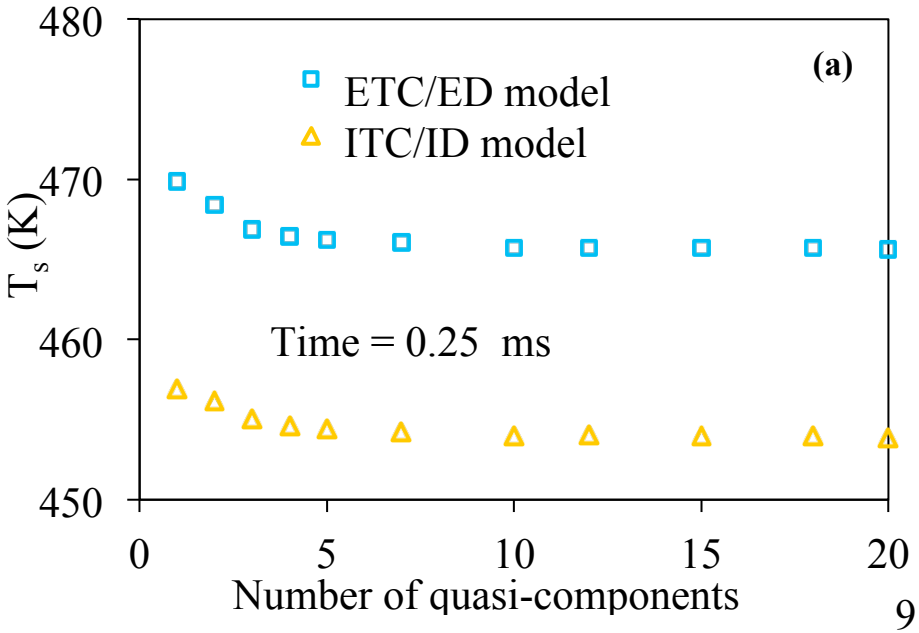
Preliminary results

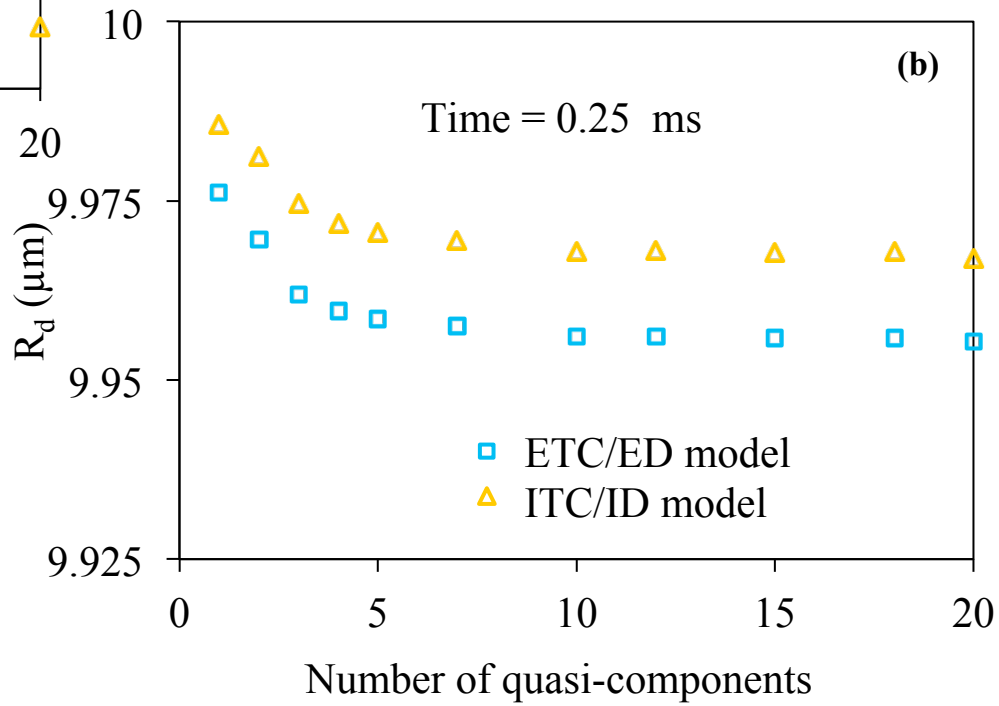
Diesel Results



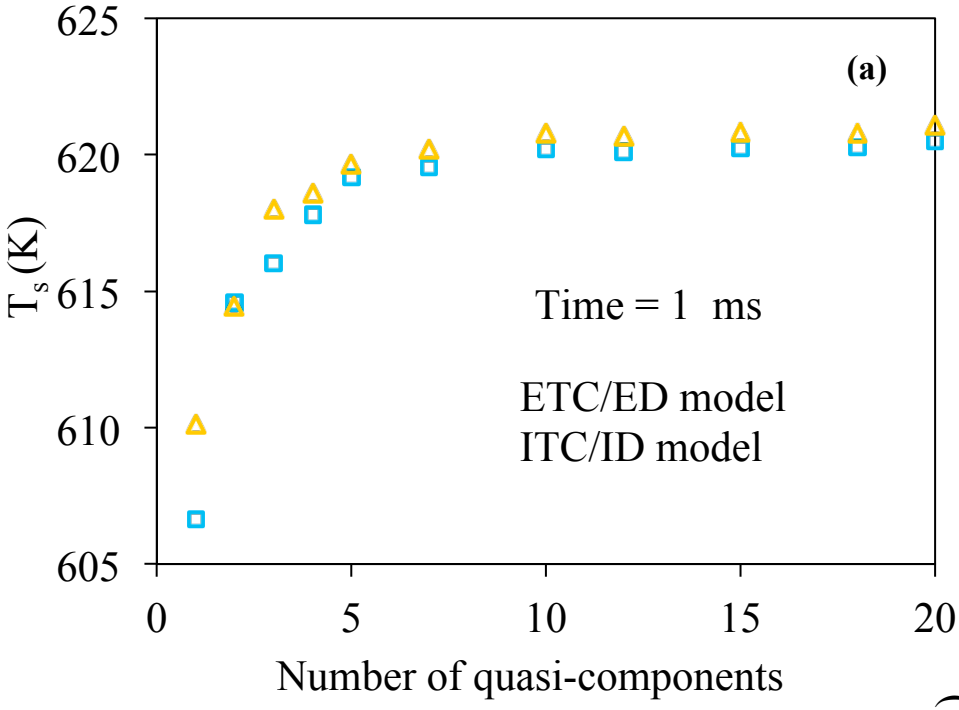
P_g =3 Mpa, R_d =10 μm, U_d =1 m/s,T_g = 880 K, $T_{d,initial}$ = 300 K

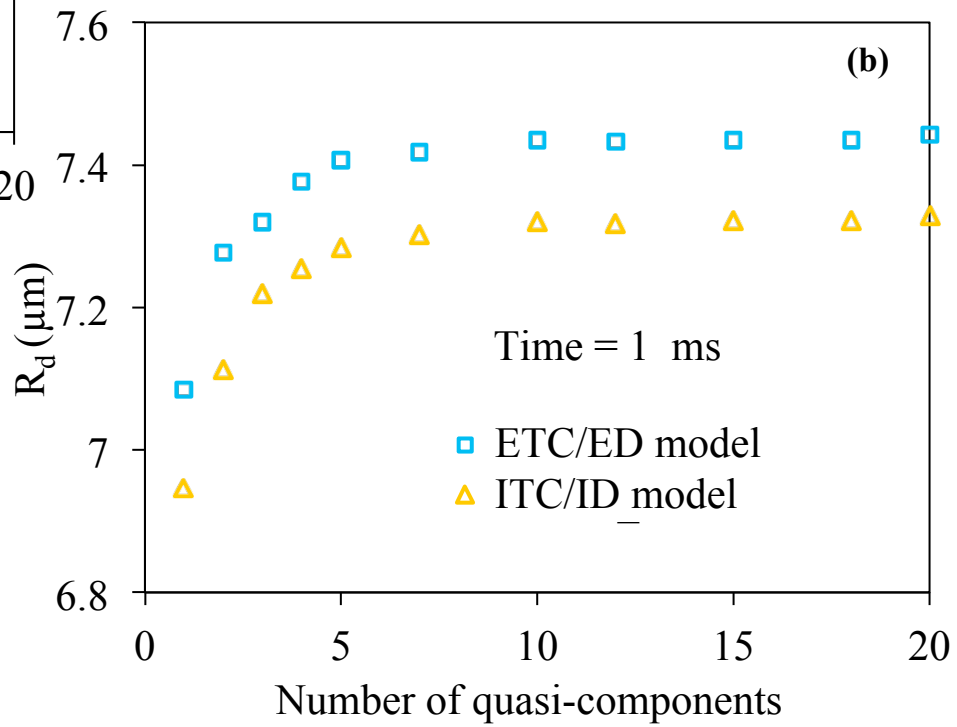
Diesel Results





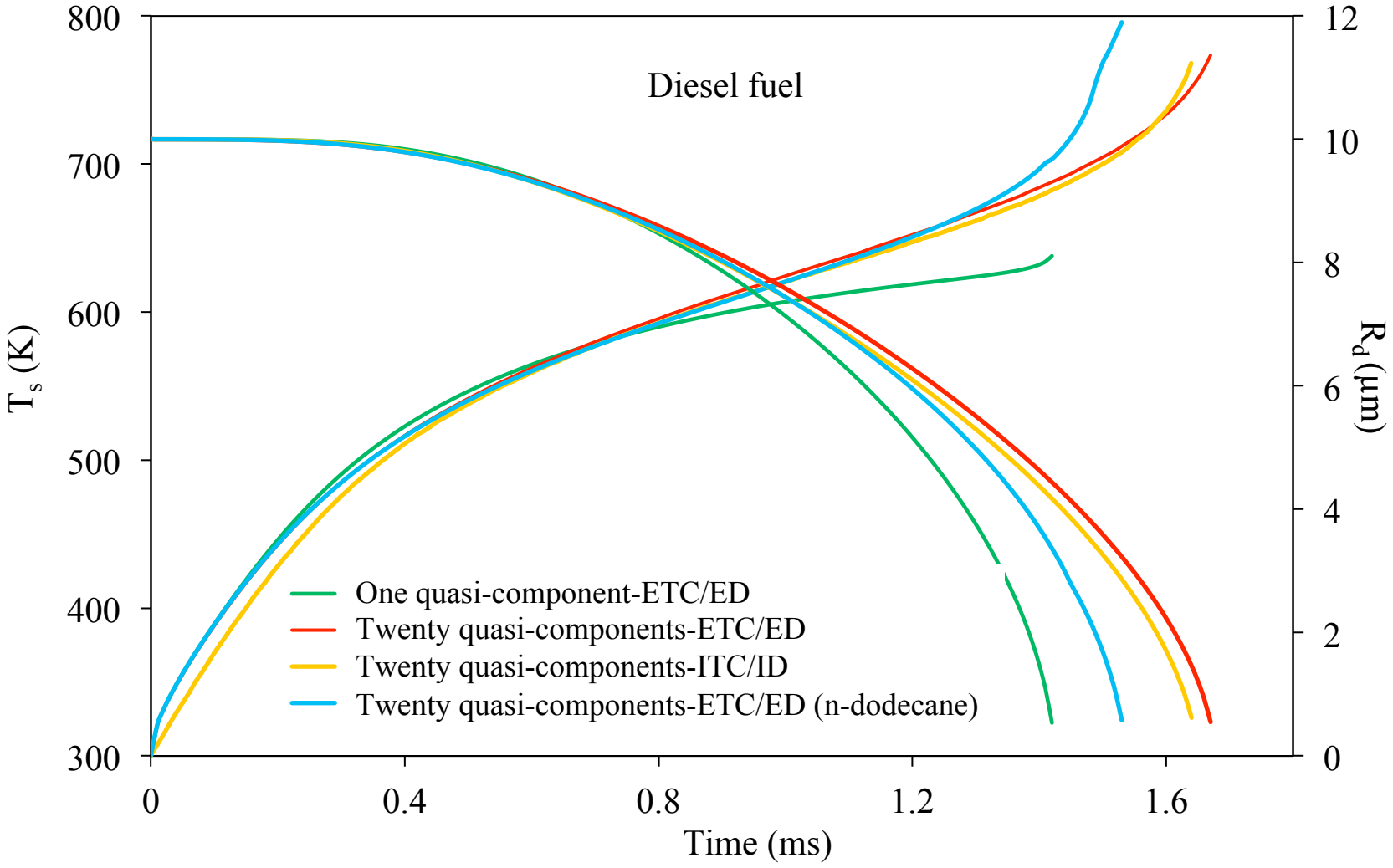
Diesel Results





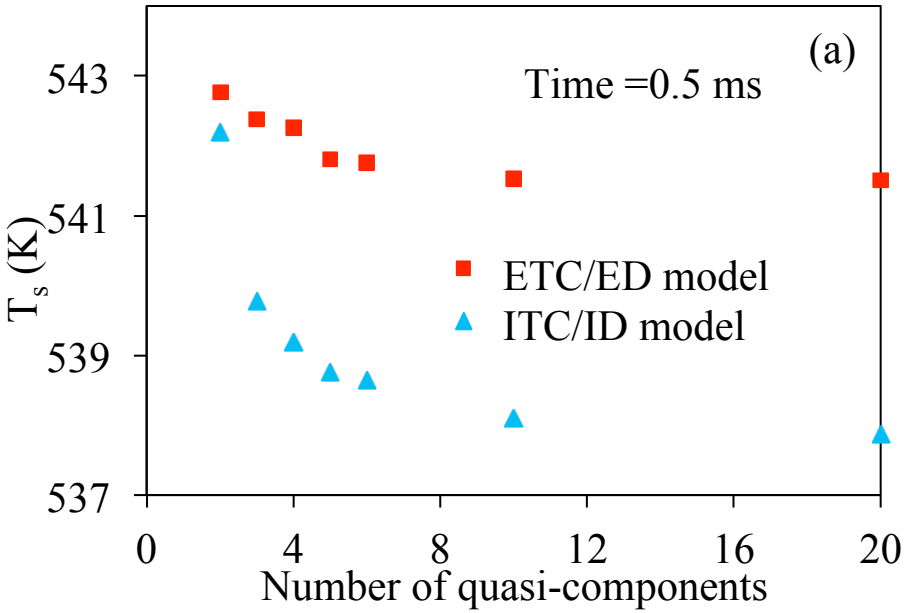
Advanced results

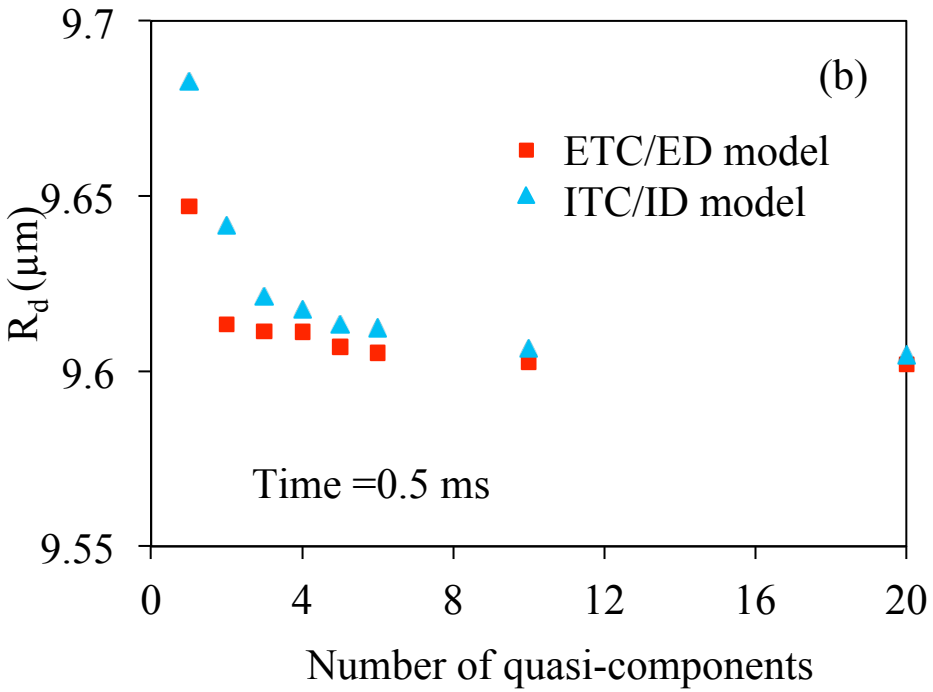
Diesel Results



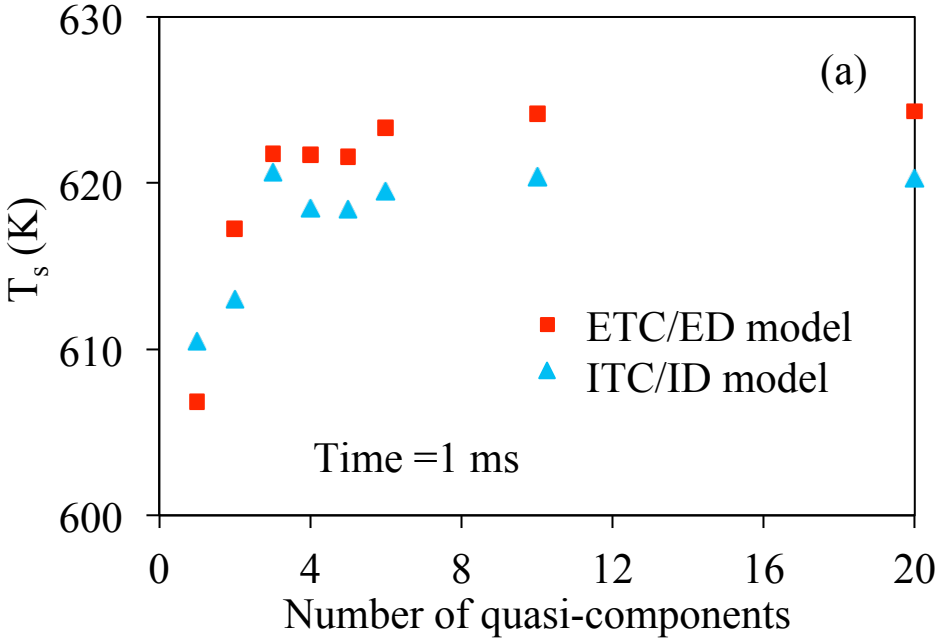
P_g =3 Mpa, R_d =10 μm, U_d =1 m/s,T_g = 880 K, $T_{d,initial}$ = 300 K

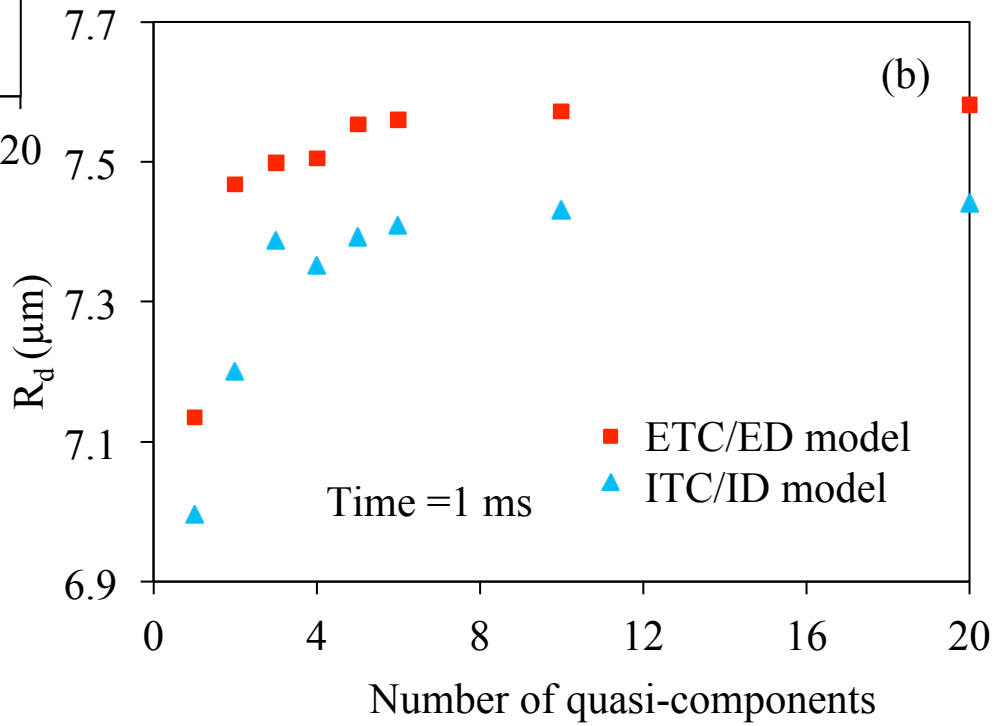
Diesel Results



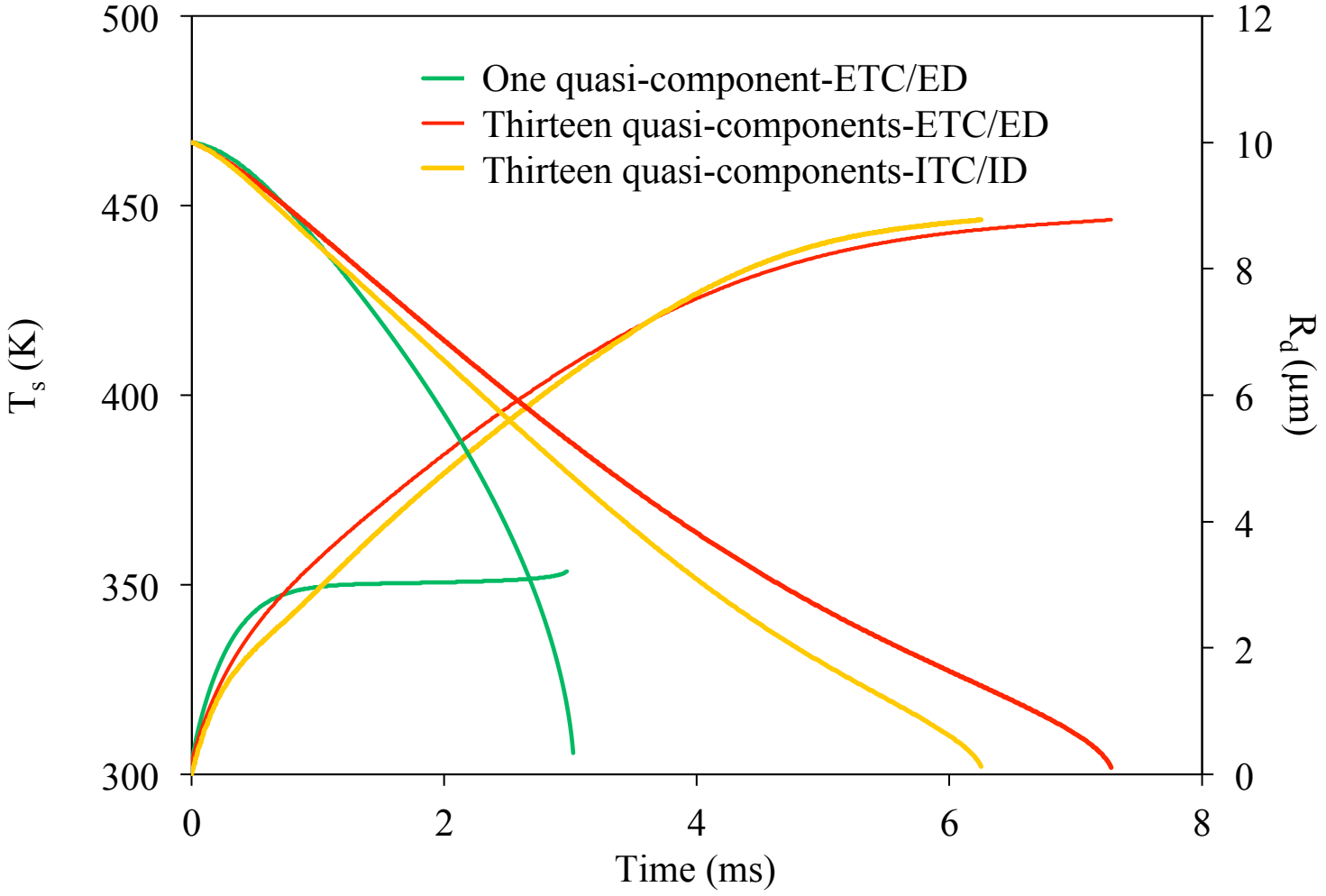


Diesel Results



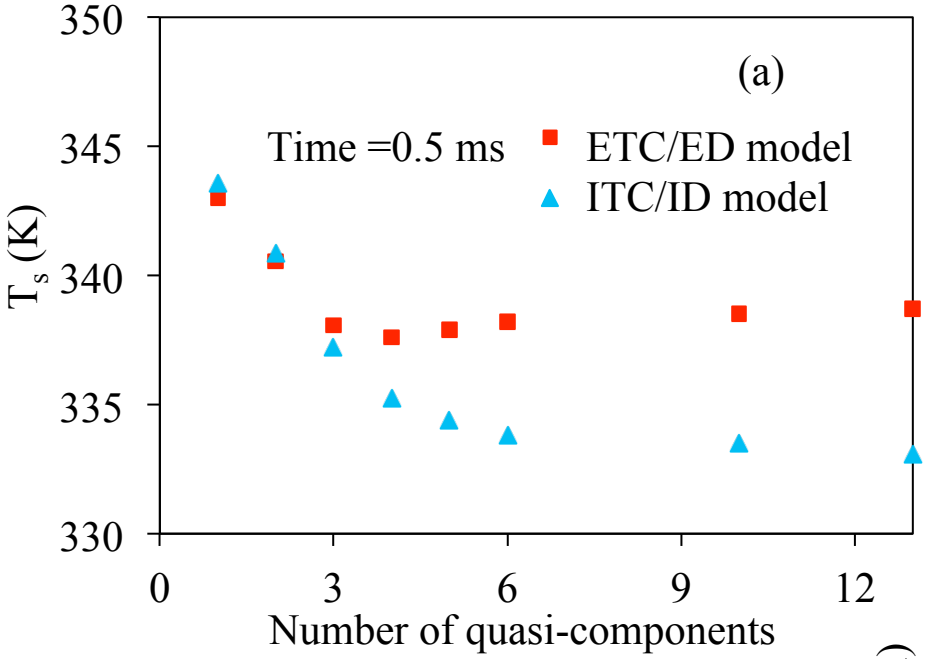


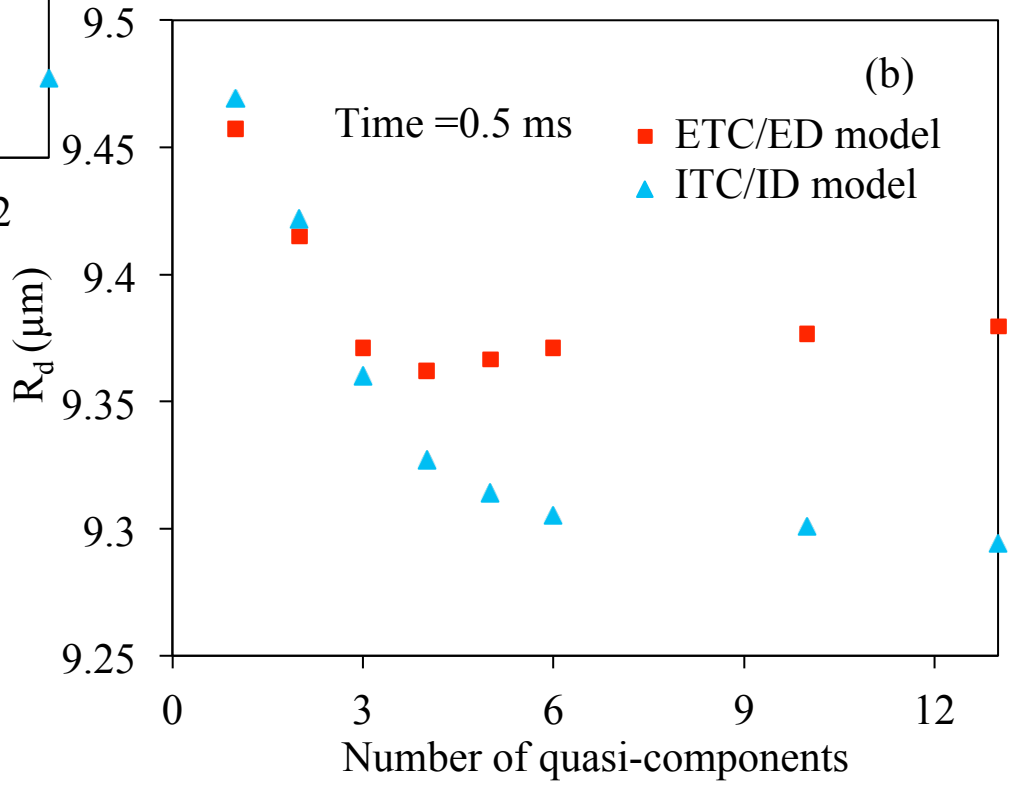
Gasoline Results



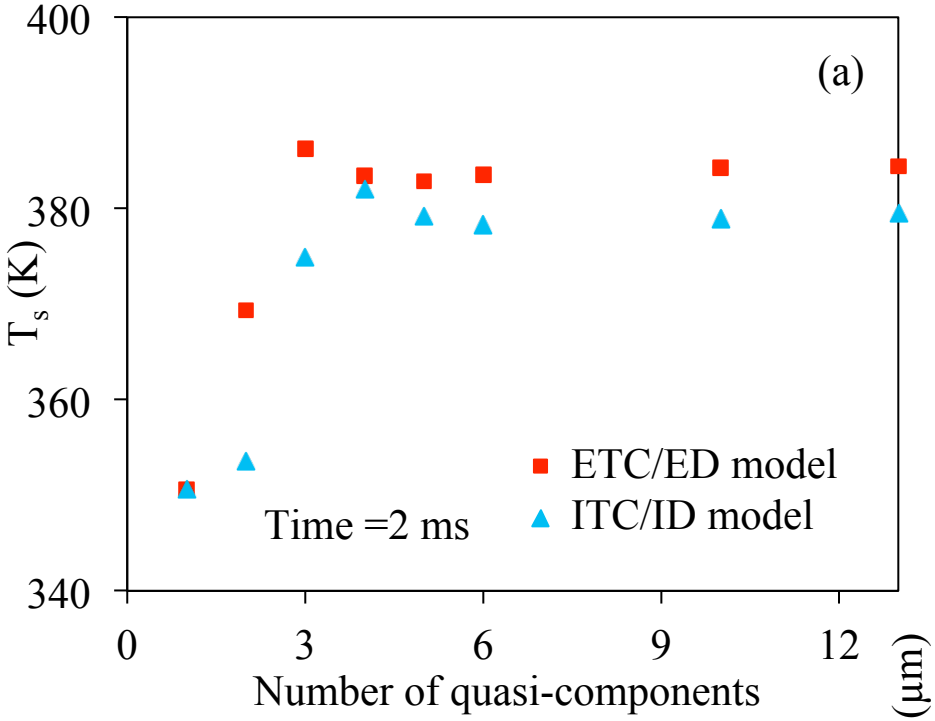
P_g =3 bar, R_d =10 μm, U_d =10 m/s,T_g = 450 K, $T_{d,initial}$ = 300 K

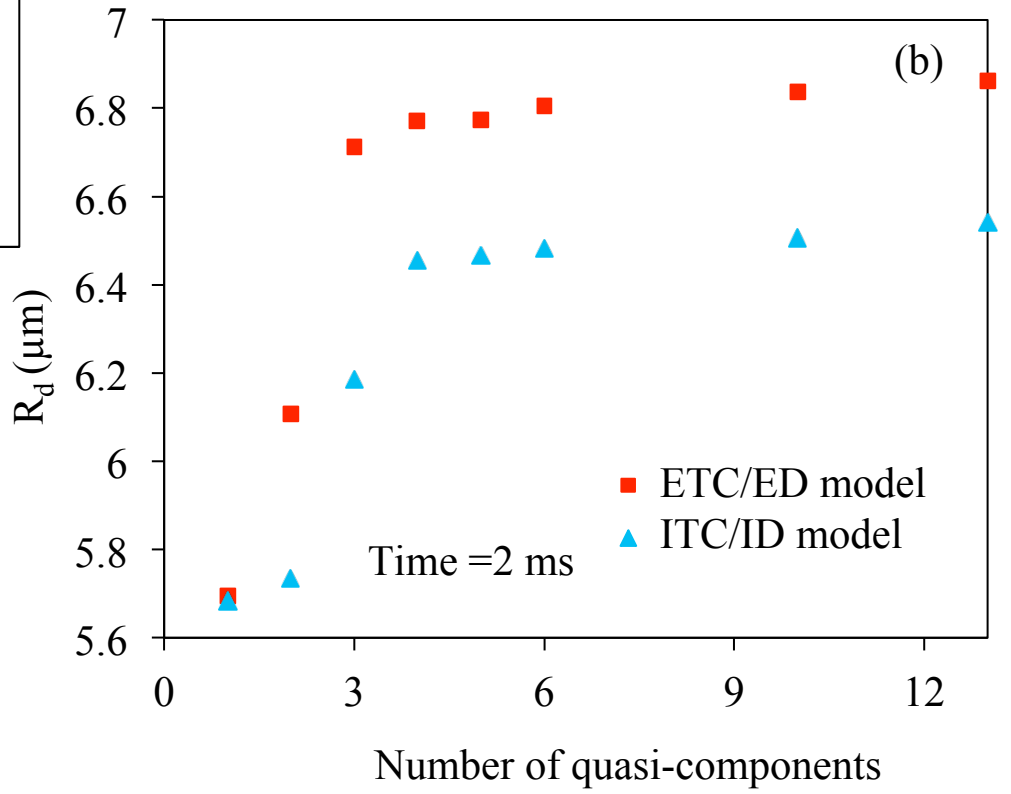
Gasoline Results





Gasoline Results





Suggested composition for Diesel and gasoline fuels

Gasoline Fuel	Diesel Fuel
60% C_6H_{14}	10% C_8H_{18}
30% C_9H_{20}	57% $C_{12}H_{26}$
8% $C_{12}H_{26}$	29% $C_{16}H_{34}$
3% $C_{15}H_{32}$	4% $C_{21}H_{44}$

Conclusions

- A new quasi-discrete model for multi-component droplets heating and evaporation, applicable for large number of components, has been developed.

- This model takes into account the effect of heat and mass diffusion within the droplet and it takes into account the dependence of the thermophysical properties of the fuel on the number of carbon atoms and temperature.

- We applied this model for Diesel and gasoline fuels.

- Diesel and Gasoline fuels could be presented by a mixture of only four quasi-components.

Publications: International Journals

- Kristyadi T., Deprédurand V., Castanet G., Lemoine F., Sazhin S.S., Elwardany A., Sazhina E.M. and Heikal M.R. (2010), *Monodisperse monocomponent fuel droplet heating and evaporation*, Fuel 89 (2010) 3995–4001.

- Sazhin S.S., Elwardany A.E., Krutitskii P.A., Castanet G., Lemoine F., Sazhina E.M. and Heikal M.R. (2010), *A simplified model for bi-component droplet heating and evaporation*, Int. J. Heat Mass Transfer 53, 4495–4505.

- Abdelghaffar, W.A., Elwardany, A.E., Sazhin, S.S. (2011), *Modelling of the processes in Diesel engine-like conditions: effects of fuel heating and evaporation*, Atomization and Sprays, 53(13-14), 2826-2836.

- Sazhin S.S., Elwardany A.E., Krutitskii P.A., Deprédurand V., Castanet G., Lemoine F., Sazhina E.M., Heikal M.R. (2011), *Multi-component droplet heating and evaporation: numerical simulation versus experimental data*, Int. J. Thermal Sciences, 50(2011) 1164-1180.

- Sazhin S.S., Elwardany A.E., Sazhina E.M., Heikal M.R. (2011), *A quasi-discrete model for heating and evaporation of complex multicomponent hydrocarbons fuel droplets*, Int. J. Heat Mass Transfer 54, 19-20, 4325-4332.

Thank you

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