Biodiesel Fuel Droplets

Modelling of Heating and Evaporation Processes

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3rd meeting, August 2013

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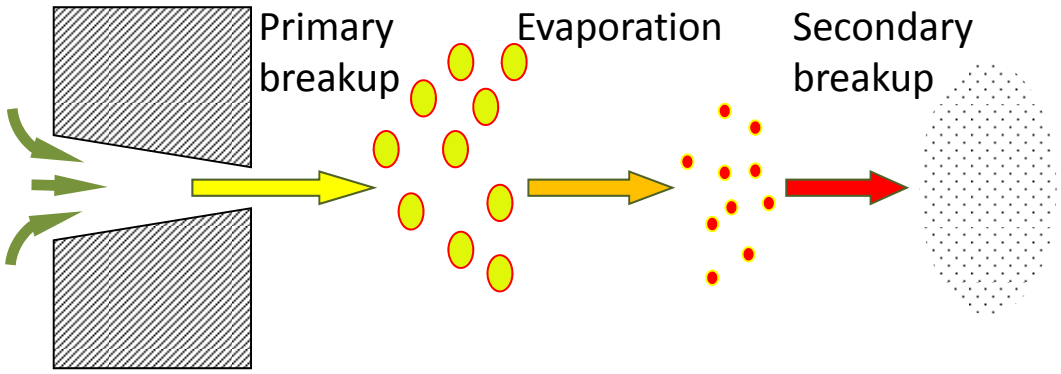
Outline

- Background
- Model
- Results
- Conclusions
- Work in progress

Processes in the Combustion Chamber of an IC Engine

- Liquid fuel jet break-up
- Droplet break-up



- Heating of droplets
- Evaporation of droplets
- Ignition and combustion

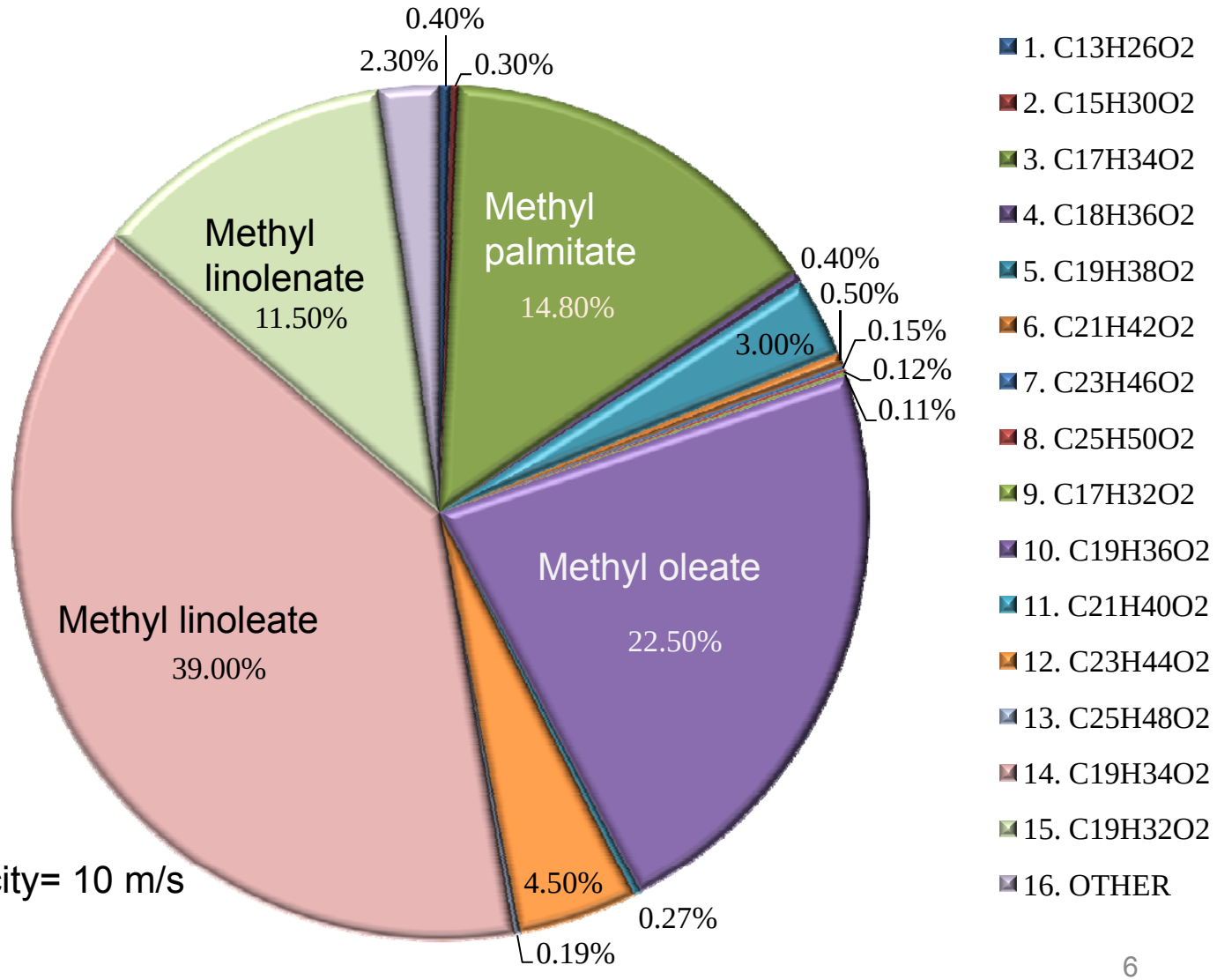
Previously Developed Models

- A model for bi-component droplets
- Effects of the moving boundary
- Quasi-discrete model (applications to n-alkanes only)

Model

- Discrete Component model (DCM).
- Each component in the fuel droplet is taken into account.
- The temperature gradient, re-circulation and species diffusion inside droplets are taken into account (Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) Model).
- The relevant Partial Differential Equations (PDEs) are solved analytically.

Biodiesel Fuel



Input parameters

- droplet radius= 12.66 μm
- temperature= 375 K
- gas pressure= 30 bar
- gas temperature=880 K
- The droplet relative velocity= 10 m/s

Basic Equations

Transient heat conduction equation:

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

$\kappa = k_{\text{eff}}/C_l\rho_l$ & k_{eff} is the effective thermal diffusivity ($k_{\text{eff}} = \chi k_l$), taking into account the recirculation effect inside droplets:

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

$\text{Pe}_{\text{d}(l)}$ is Peclet number ($\text{Pe}_{\text{d}(l)}=\text{Re}_{\text{d}(l)}\,\text{Pr}_l$) and $1 < \chi < 2.72$.

Basic Equations

Initial and boundary conditions (heat transfer):

$$\left.\begin{aligned} T(t=0) &= T_{d0}(R) \\ h\left(T_g - T_s\right) &= k_{\text{eff}} \left.\frac{\partial T}{\partial R}\right|_{R=R_d-0} \end{aligned}\right\} \quad \ldots(3)$$

T_s= droplet surface temperature, T_g= ambient gas temperature, R_d= droplet radius and h= convective heat transfer coefficient.

Eq. (1) can therefore be derived into:

$$T(R,t_1) = \frac{1}{R}\sum_{n=1}^{\infty} \left\{ \begin{aligned} & q_n \exp[-\kappa_R \lambda_n^2 t_1] - \frac{R_d^2 \sin\lambda_n}{\|v_n\|^2 \lambda_n^2} \mu_0(0) \exp[-\kappa_R \lambda_n^2 t] - \\ & \frac{R_d^2 \sin\lambda_n}{\|v_n\|^2 \lambda_n^4} \int_0^t \frac{d\mu_{0(\tau)}}{d\tau} \exp[-\kappa_R \lambda_n^2 (t-\tau)] d\tau \end{aligned} \right\} \sin\left(\lambda_n \frac{R}{R_d}\right) + T_g(t_1) \quad \ldots(4)$$

Basic Equations

Species mass transfer equation:

$$\frac{\partial Y_{li}}{\partial t} = D_{eff}\left(\frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R}\frac{\partial Y_{li}}{\partial R}\right) \quad ...(5)$$

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

$$\chi_Y = 1.86 + 0.86\tanh\left[2.225\ \log_{10}\left(\mathrm{Re}_{d(l)}\mathrm{Sc}_l/30\right)\right] \quad ...(6)$$

$(1<\chi_Y<2.72)$ and $\mathrm{Sc}_l = \frac{\nu_l}{D_l}$

Basic Equations

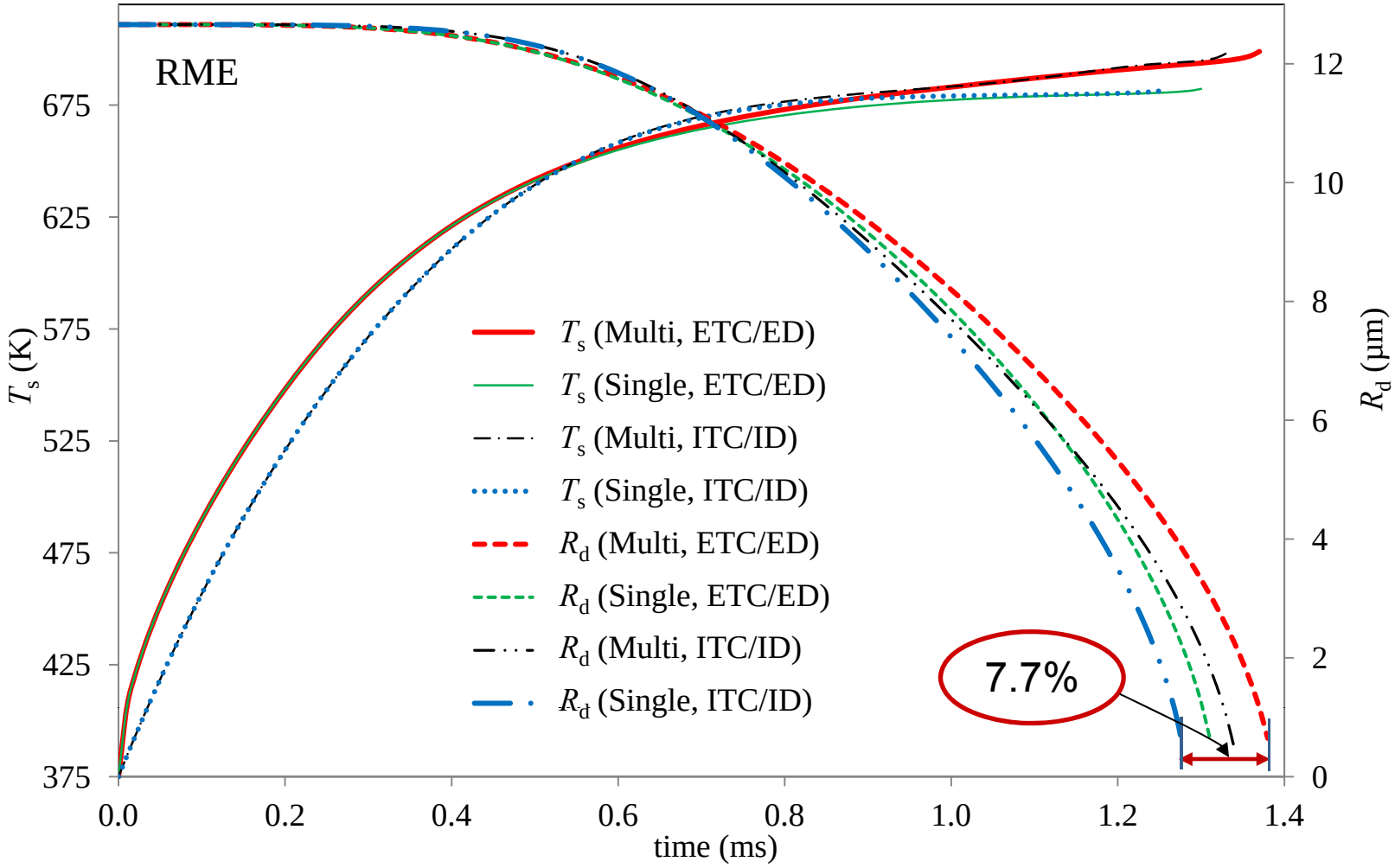
Initial and boundary conditions (evaporation):

$$\left.\begin{aligned} Y_{li}(t=0) &= Y_{li0}(R) \\ \alpha(\epsilon_i - Y_{lis}) &= -D_{eff}\left.\frac{\partial Y_{li}}{\partial R}\right|_{R=R_d-0} \end{aligned}\right\} \quad \ldots(9)$$

Y_{lis}= mass fraction, □$_i$= evaporation rate of each component and □ fixed factor for all components, $\alpha = |\dot{m}_d|/(4\pi\rho_l R_d^2)$. Solution to Eq. (5) :

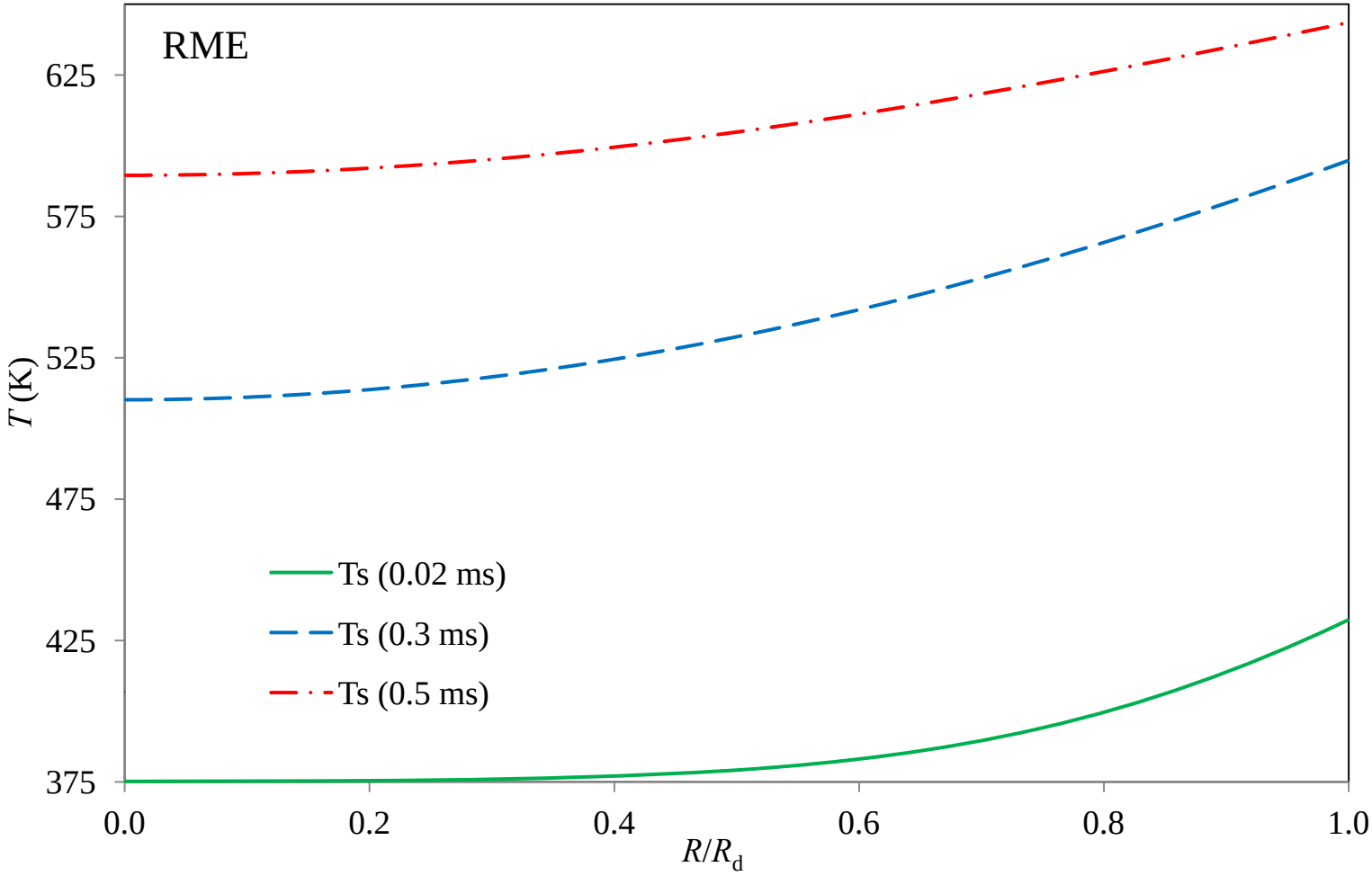
$$Y_{li} = \epsilon_i + \frac{1}{R}\left\{\begin{aligned} &\left[\exp\left[D_{eff}\left(\frac{\lambda_0}{R_d}\right)^2 t\right]\right][q_{i0} - \epsilon_i Q_0]\sinh\left(\lambda_0\frac{R}{R_d}\right) + \\ &\sum_{n=1}^{\infty}\left[\exp\left[-D_{eff}\left(\frac{\lambda_n}{R_d}\right)^2 t\right]\right][q_{in} - \epsilon_i Q_n]\sin\left(\lambda_n\frac{R}{R_d}\right) \end{aligned}\right\} \quad \ldots(10)$$

Surface Temperature and Radius



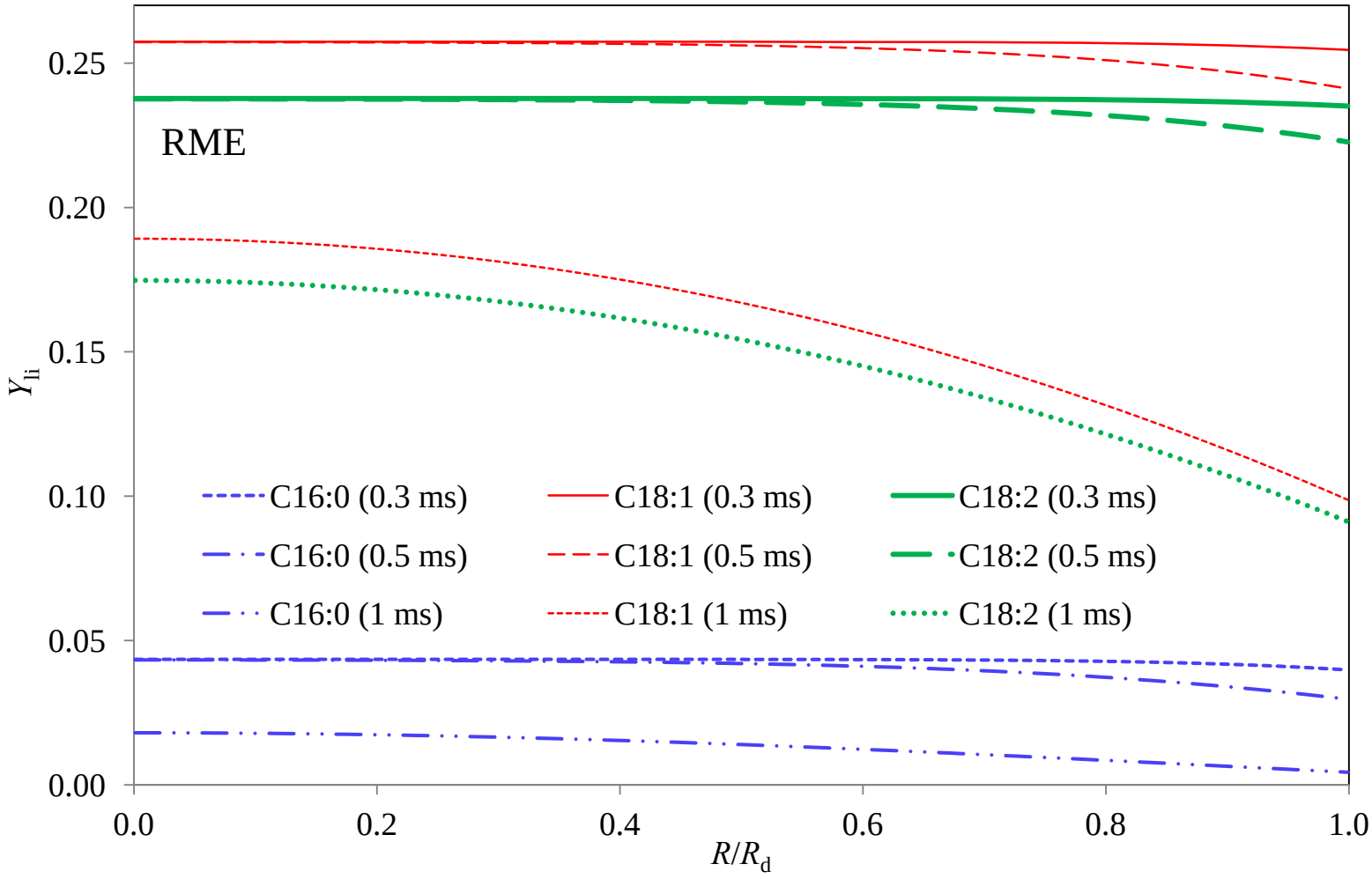
The time evolution of Rapeseed Methyl Ester (RME) droplet surface temperatures (T_s) and radii (R_d) predicted by ED/ETC, ID/ITC, single- and multi-component models

Temperature Gradient



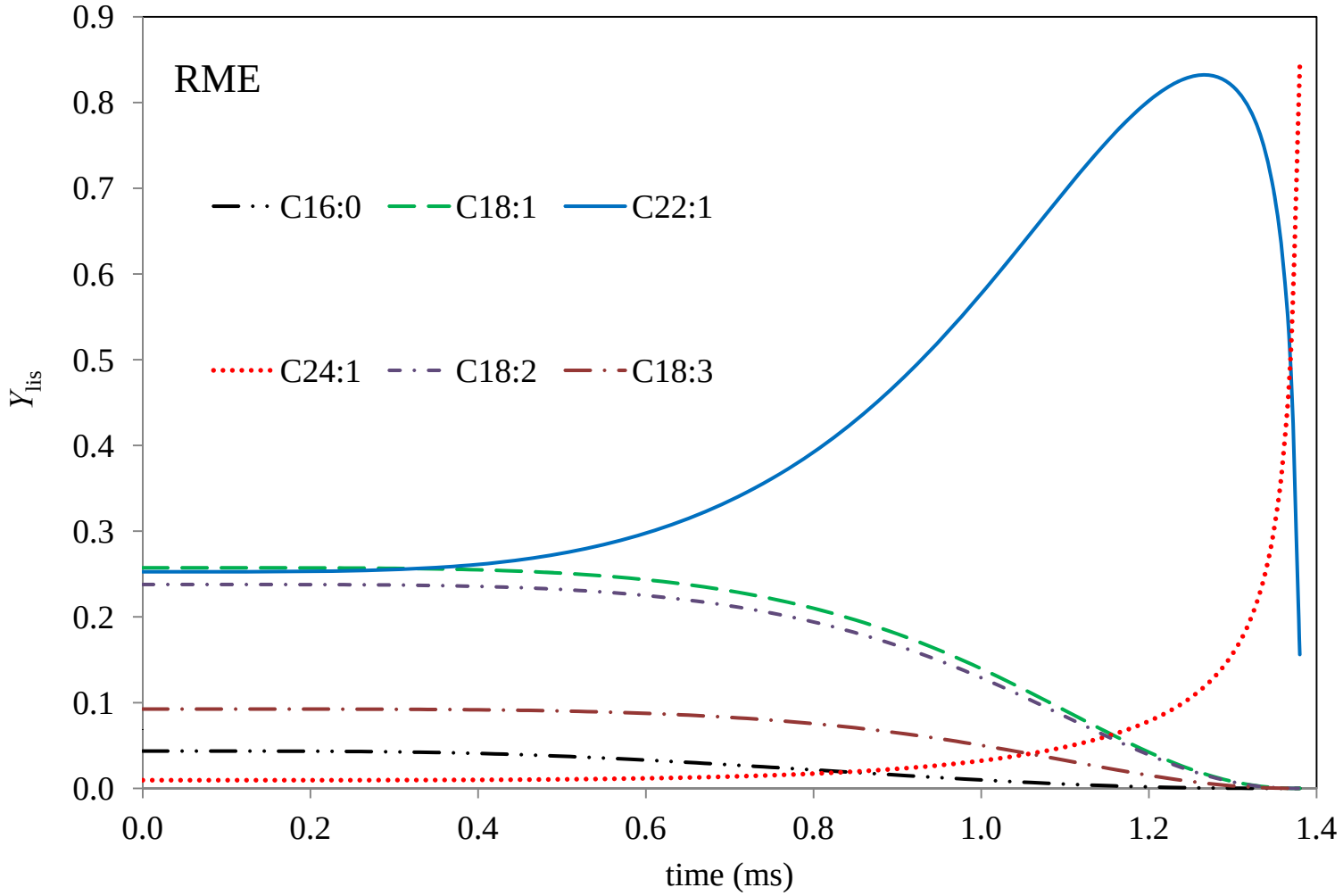
The temperature T versus R/R_d at 3 time instants, 0.02 ms, 0.3 ms and 0.5 ms, predicted by the ETC/ED model

Mass Fractions inside the Droplet



The species mass fraction Y_{li} versus R/R_d at 3 time instants (0.3 ms, 0.5 ms and 1 ms) predicted by the ETC/ED model

Surface Mass Fractions



Liquid species mass fractions at the droplet surface Y_{lis}, for six RME dominant components versus time

Conclusions

- The mono-component model leads to errors in predicted droplet evaporation time of up to 5.5% and surface temperatures of up to 2.4% compared with the prediction of the multi-component model.

- Using ID/ITC model and mono-component approximation leads to a deviation in the predicted evaporation time of up to 7.7%.

Work in Progress

- The generalisation of the multi-component model for the applications to real industrial fuels (Diesel and gasoline fuels)

- The implementation of the models into a commercial CFD code for wider industrial applications

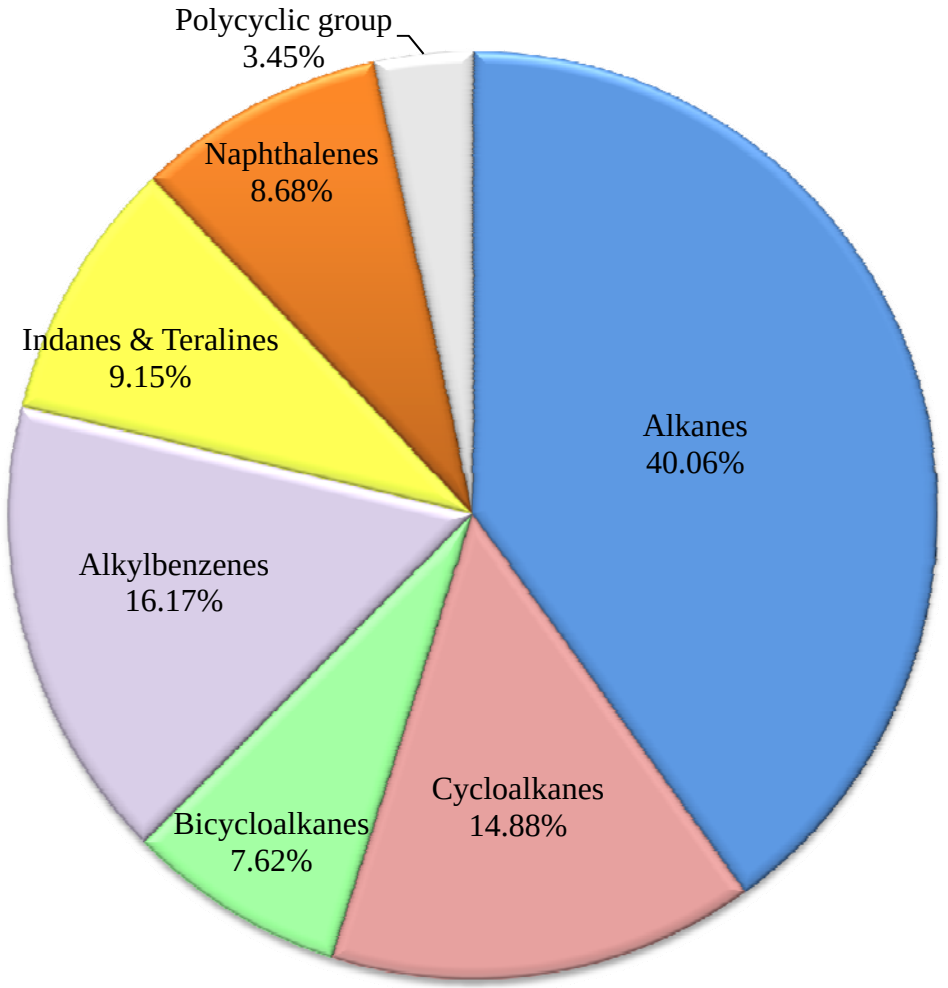
Quasi-Discrete Model

- The model is based on replacing the large number of actual components with a small number of quasi-components
- These quasi-components are treated as actual components in this model, taking into account the diffusion of quasi-components in droplets

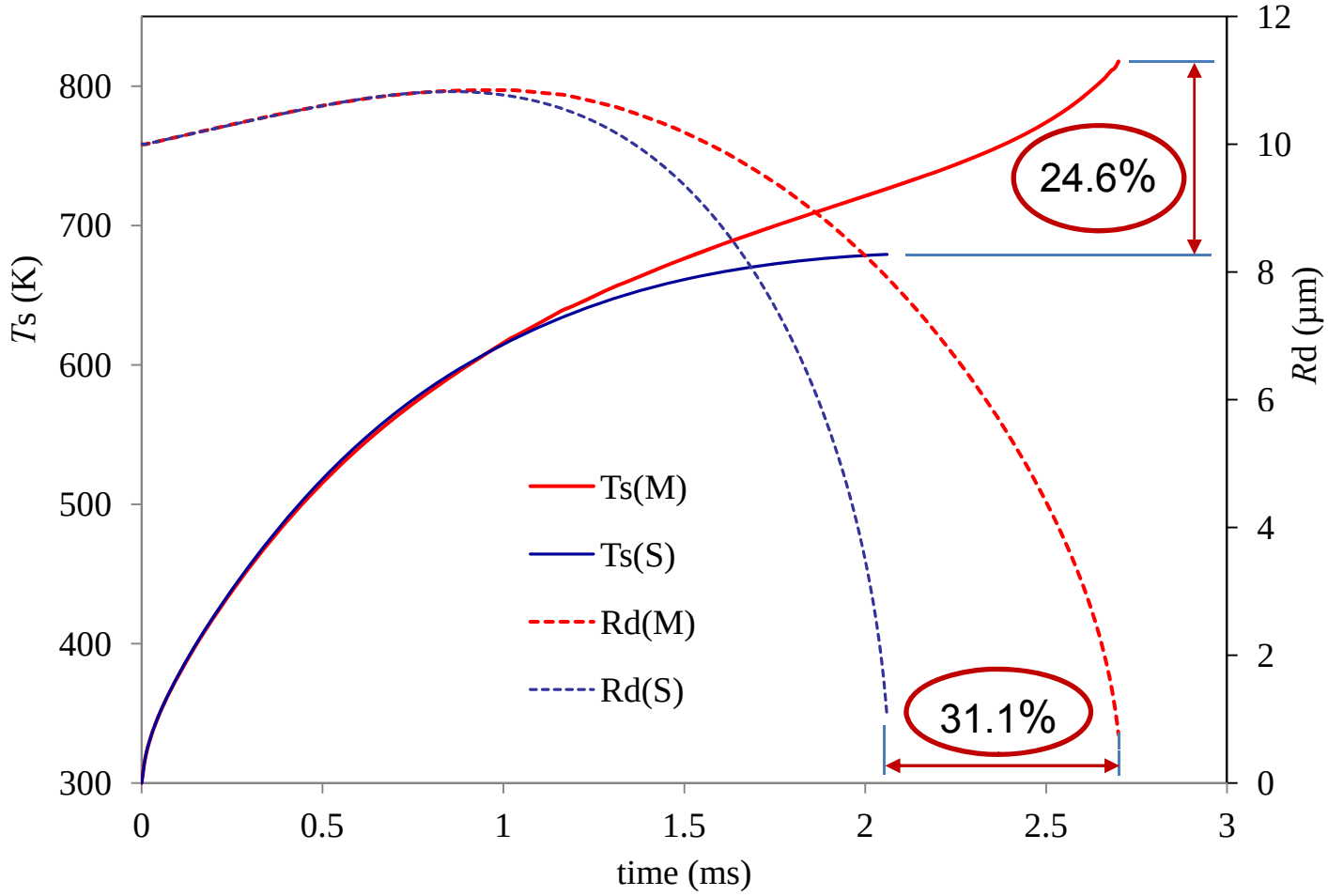
Realistic Diesel Fuel

Input parameters

- droplet radius= 10 μm
- temperature= 300 K
- gas pressure= 30 bar
- gas temperature=880 K
- the droplet relative velocity= 0
- each group contains up to 20 components



Preliminary Results



The time evolution of surface temperatures (T_s) and radii (R_d) predicted by single- and multi-component models

Conclusions

- The mono-component model leads to errors in predicted droplet evaporation time of about 31.1% and surface temperatures of up to 24.6% compared with the prediction of the multi-component model for Diesel groups.

- The increase in errors of realistic Diesel fuel compared to biodiesel fuel is related to the high number of components and contribution effect on the droplet heating evaporation.

Thank you!

Your Comments would be highly appreciated..

Resources

Al Qubeissi, M., Kolodnytska, R. and Sazhin, S.S. (2013) Biodiesel Fuel Droplets: Modelling of Heating and Evaporation Processes. *Proceedings of Ilass-Europe 25th, Chania, Greece* (in press).

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Further helpful notes

What is Biodiesel Fuel?

Biodiesel refers to fuels comprised of mono-alkyl esters of long-chain fatty acids derived from vegetable oils or animal fats, including waste oil

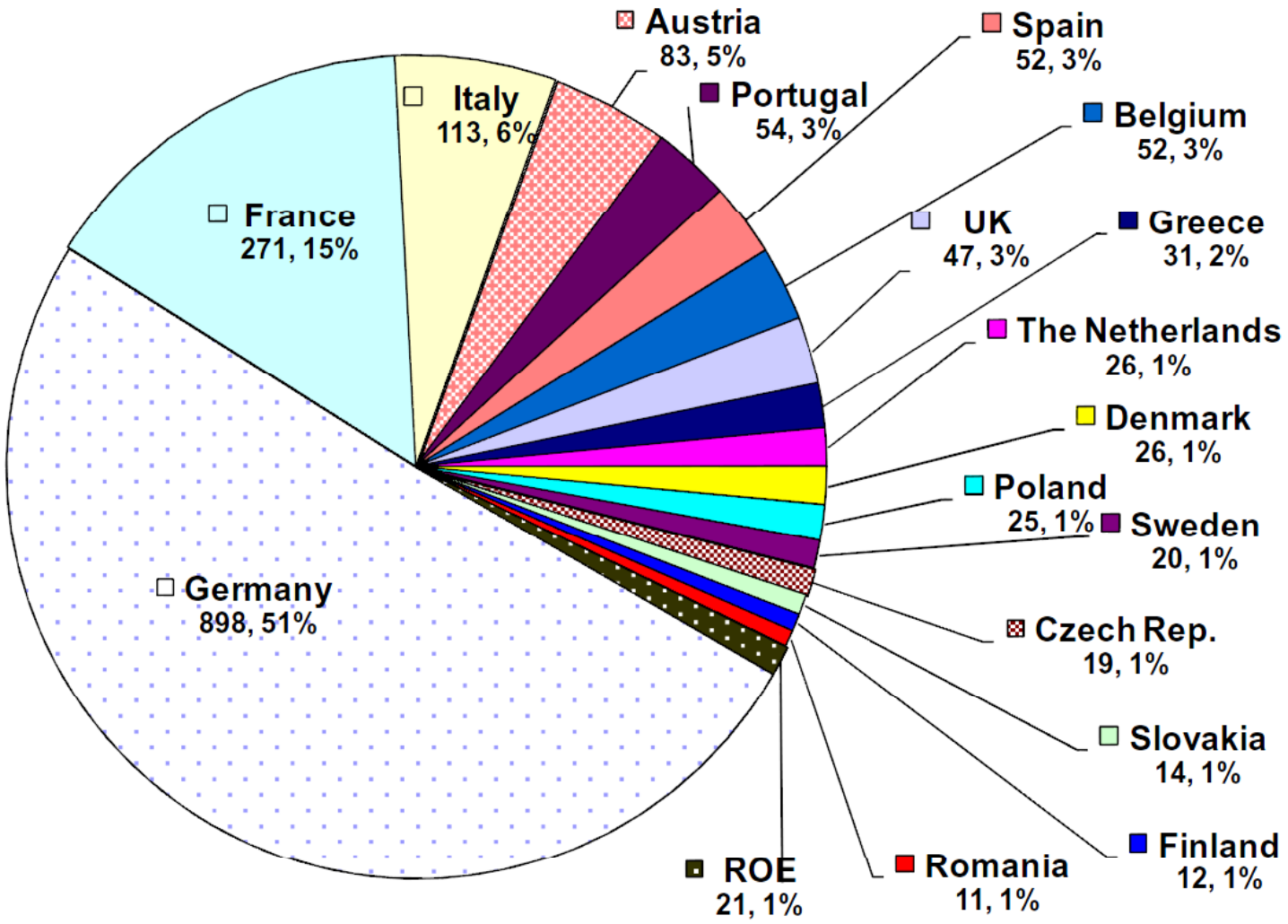
Biodiesel fuels used

- Palm Methyl Ester (PME), from palm seed oil
- Hemp Methyl Esters, from hemp seed oil, the Ukrainian (HME1) and the E.U. (HME2)
- Rapeseed Methyl Ester (RME), from rapeseed oil
- Soybean Methyl Ester (SME), from soybean oil

Why Modelling Biodiesel Fuel?

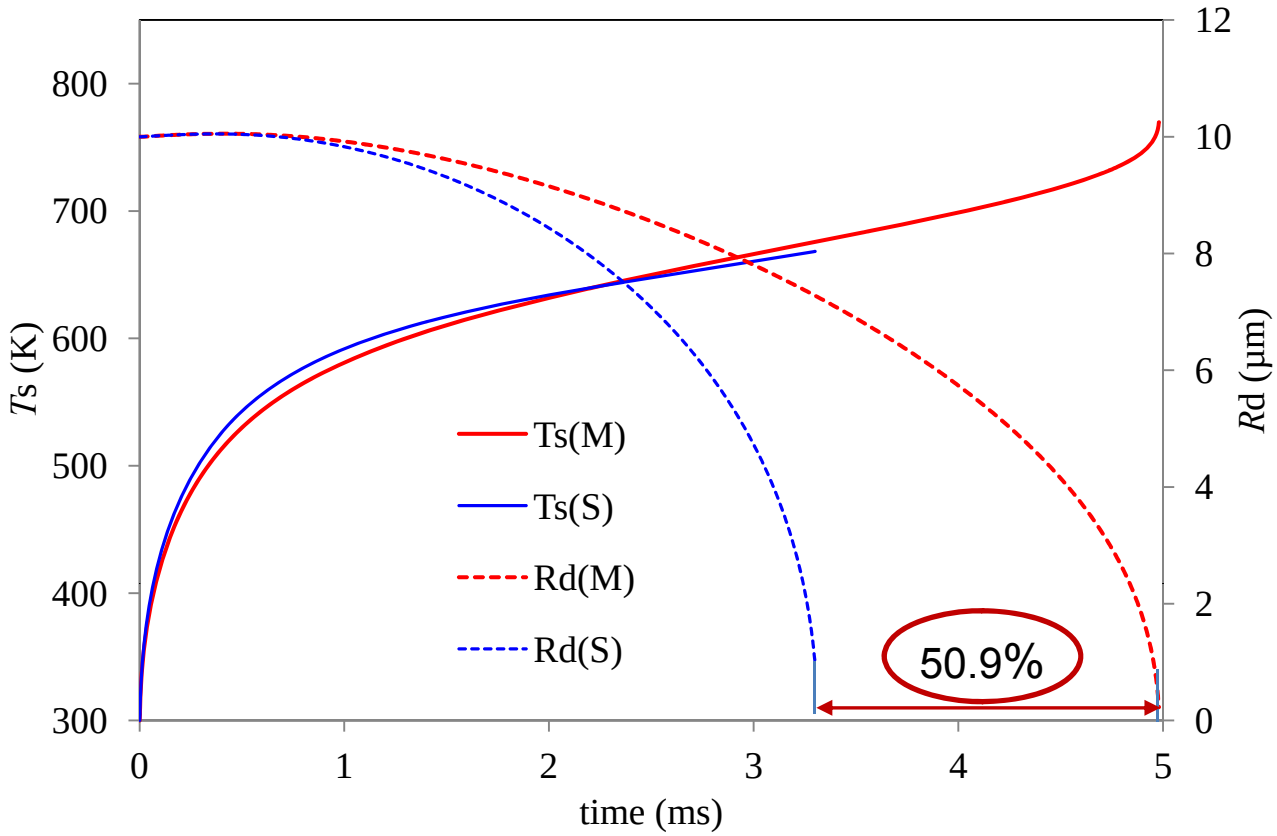
- More efficient alternative (typically 40% higher MPG than petroleum)
- Clean burning alternative (80% less carbon dioxide & 100% less sulphur dioxide)
- Higher life expectancy for engine (far more lubricant than diesel)
- Can be used in compression-ignition engines with little/no modifications
- Easy to use, produce and recycle
- It can instigate economic growth and job creation by establishing feedstock plantations

European Production of Biodiesel (2007)*



* Courtesy of *SAE Int. J. Fuels Lubr., Vol. 2, Issue 2, 185-232.*

Preliminary Results (Indanes & teralines)



The time evolution of surface temperatures (T_s) and radii (R_d) predicted by single- and multi-component models for a droplet formed of indanes and tetralines only