# Modelling of heating and evaporation of kerosene droplets

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# Plan

Background

Kerosene droplets

Surrogate droplets

Final thoughts

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# Background

# Dimensionless numbers

Biot number

$$\mathrm{Bi} = \frac{2\, h R_d^2}{k_l}$$

# Dimensionless numbers

Biot number

**Fourier number**

$$\text{Bi}= \frac{2\,hR_d^2}{k_l}$$

$$\text{Fo} = \frac{k_l\, t}{c_l \rho_l R_d^2}$$

# Effective thermal conductivity (spherical droplets)

$$c_l \rho_l \frac{\partial T}{\partial t} = k_{\mathrm{eff}} \left( \frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right) + P_1(R)$$

$P_1(R)$ is the power generated per unit volume inside the droplet due to thermal radiation

Boundary and initial conditions:

$$h\left(T_{g\infty} - T_s\right) = k_{\mathrm{eff}} \frac{\partial T}{\partial R}\Big|_{R=R_R}$$

$$\frac{\partial T}{\partial R}\Big|_{R=0} = 0; \quad T(t=0) = T_0(R); \qquad R \leq R_d$$

Effective thermal conductivity $k_{\mathrm{eff}} = \chi k_l$ where $\chi = 1.86 + 0.86 \tanh\left[2.225 \log_{10}(\mathrm{Pe}_d/30)\right]$

$\chi$ increases from 1 to 2.72 when $\mathrm{Pe}_d = \mathrm{Re}_{ds} \mathrm{P}r_d$ increases from <10 to > 500

# Discrete components model (spherical droplets)

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

Boundary and initial conditions:

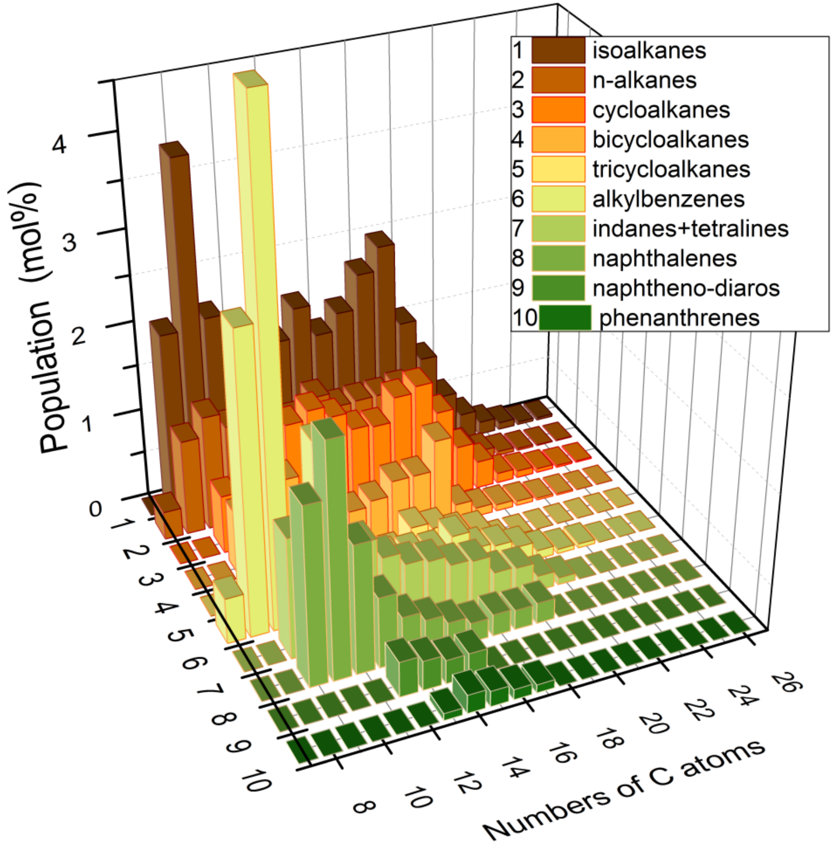
$$\alpha(\epsilon_i - Y_{lis}) = D_{\text{eff}}\frac{\partial Y_{li}}{\partial R}\Big|_{R=R_R-0}$$

$$\frac{\partial Y_{li}}{\partial R}\Big|_{R=0} = 0;\ \ Y_{li}\,(t=0) = Y_{li0}\,(R); \quad R \leq R_d$$

Effective diffusivity $D_{\text{eff}}=\chi_Y D_l$ where $\chi_Y=1.86+0.86\tanh\left[2.225\log_{10}(\text{Pe}_{dY}/30)\right]$

$\chi_Y$ increases from 1 to 2.72 when $\text{Pe}_{dY}=\text{Re}_d Sc$ increases from <10 to > 500

$\text{Sc}=\nu_l/D_l$ is the liquid Schmidt number; $\epsilon_i = \frac{Y_{vis}}{\sum_i Y_{vis}}$ $\quad \alpha = \frac{|\dot{m}_d|}{4\pi\rho_l R_d^2}$




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 |

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


Fuel 129 (2014) 238–266

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A multi-dimensional quasi-discrete model for the analysis of Diesel fuel droplet heating and evaporation


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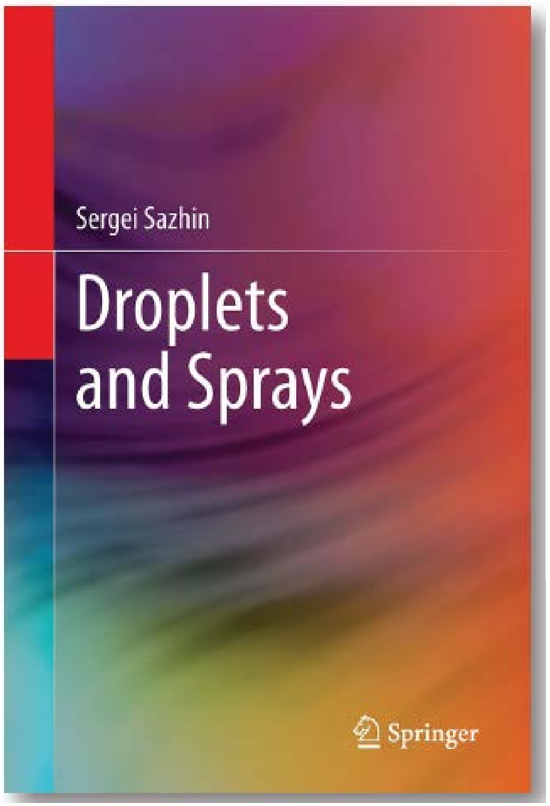


Fuel 196 (2017) 69–101

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Review article

# Modelling of fuel droplet heating and evaporation: Recent results and unsolved problems

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# Kerosene droplets

# Kerosene composition

| CN | Par | Na/Ol | Alk | Napht | Dia |
|---|---|---|---|---|---|
| C7 | 0.4100 | 0.1700 | 0.0900 | 0 | 0 |
| C8 | 0.5800 | 0.6300 | 0.6100 | 0 | 0 |
| C9 | 2.2100 | 2.3700 | 1.5600 | 0.2200 | 0 |
| C10 | 4.7900 | 5.8300 | 2.7200 | 1.0600 | 0.0900 |
| C11 | 6.0900 | 6.9300 | 2.1900 | 1.8100 | 0.2500 |
| C12 | 7.5200 | 7.4000 | 3.0000 | 3.4800 | 0.3000 |
| C13 | 5.9300 | 4.4900 | 2.9100 | 0.9000 | 0.0600 |
| C14 | 6.0300 | 3.7800 | 1.7400 | 0.2400 | 0 |
| C15 | 6.2100 | 1.6700 | 0.3500 | 0 | 0 |
| C16 | 2.1600 | 0.7400 | 0 | 0 | 0 |
| C17 | 0 | 0.4800 | 0 | 0 | 0 |

Table 1: Mass fractions of the components of kerosene sample K1 in percent, inferred from Table 6 of [16]. CN stands for carbon number, Par for paraffins, Na/Ol for naphthenes/olefins, Alk for alkylbenzene, Napht for naphtobenzene, Dia for diaromatics

K. Lissitsyna, S. Huertas, L. C. Quintero, L. M. Polo, Piona analysis of kerosene by comprehensive two-dimensional gas chromatography coupled to time of flight mass spectrometry, Fuel 116 (2014) 716 – 722.

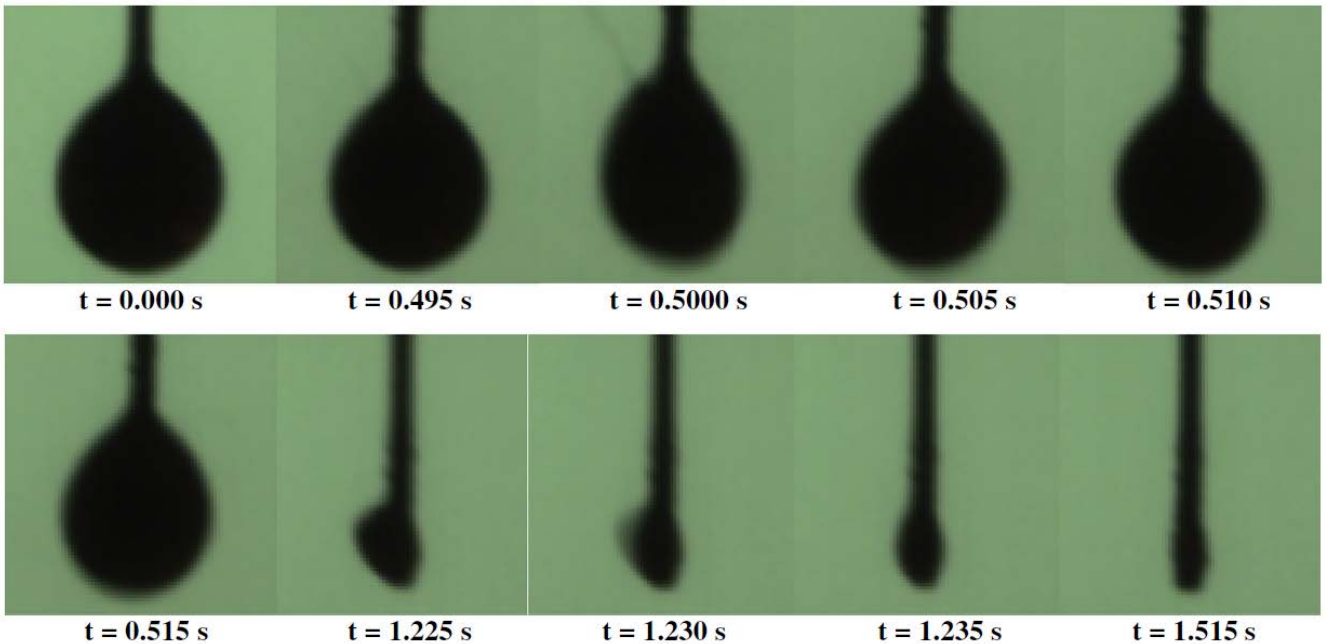
# Kerosene composition (revised)

| CN | Alk | Cycloalk | Alkyb | Ind & Tet | Naph |
|---|---|---|---|---|---|
| C7 | 0.6666 | 0.2820 | 0.1590 | 0 | 0 |
| C8 | 0.8272 | 0.9145 | 0.9356 | 0 | 0 |
| C9 | 2.8071 | 3.0581 | 2.1136 | 0.3031 | 0 |
| C10 | 5.4843 | 6.7705 | 3.3002 | 1.3056 | 0.1143 |
| C11 | 6.3470 | 7.3163 | 2.4058 | 2.0156 | 0.2862 |
| C12 | 7.1920 | 7.1614 | 3.0108 | 3.5362 | 0.3126 |
| C13 | 5.2398 | 4.0110 | 2.6882 | 0.8410 | 0.0574 |
| C14 | 4.9514 | 3.1355 | 1.4889 | 0.2076 | 0 |
| C15 | 4.7625 | 1.2929 | 0.2789 | 0 | 0 |
| C16 | 1.5539 | 0.5371 | 0 | 0 | 0 |
| C17 | 0 | 0.3279 | 0 | 0 | 0 |
| Total | 39.8 | 34.8 | 16.4 | 8.2 | 0.8 |

Table 2: Molar fractions of the components of kerosene sample K1 (in percent), inferred from Table 1 and additional assumptions described in the paper. CN stands for carbon number, Alk stands for alkanes, Cycloalk stands for cycloalkanes, Alkyb stands for alkylbenzenes, Ind & Tet for indanes & tetralines, Naph for naphthalenes.

# Kerosene droplets

I. Javed et al. / Combustion and Flame 160 (2013) 2955–2963

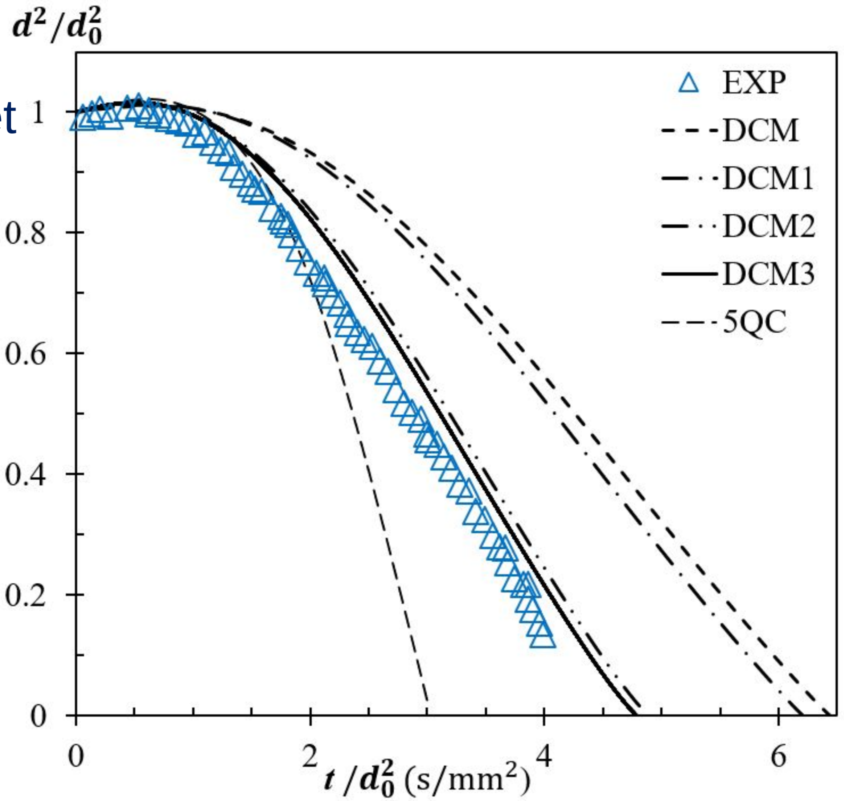


# Kerosene droplets

The initial average diameter of a droplet
1.0 ± 0.10 mm

The ambient gas temperature
T (gas)= 500 C

Experimental data from
Javed et al (2013)
Combustion and flame




The following models considered:
Discrete Component Model (DCM)
DCM as above and the contribution of supporting fibre (plots DCM1);
DCM as above accounting for natural convection (plots DCM2);
DCM as above accounting for natural convection and supporting fibre (plots DCM3);
5 Quasi components, Multi-Dimensional Quasi-Discrete Model (5QC)

# Surrogate droplets

# Surrogate droplets

| Surr. | $n-$ or **iso-** Alkanes | Cycloalkanes | Alkybenzene | Ind, Tet & Naph |
|---|---|---|---|---|
| 1 | 100% of $C_{10}H_{22}$ | 0 | 0 | 0 |
| 2 | 57.6923% of $C_{12}H_{26}$ | 19.7436% of $C_7H_{14}$ | 22.5641% of $C_8H_{10}$ | 0 |
| 3 | 46.4229% of $C_{10}H_{22}$ | 26.0095% of $C_{10}H_{20}$ | 27.5676% of $C_{10}H_{14}$ | 0 |
| 4 | 30.8611% of $C_{10}H_{22}$ | 33.5642% of $C_{10}H_{20}$ | 35.5748% of $C_{10}H_{14}$ | 0 |
| 5 | 76.9231% of $C_{10}H_{22}$ | 0 | 23.0769% of $C_6H_6$ | 0 |
| 6 | 77.6398% of $C_{12}H_{26}$ | 0 | 22.3602% of $C_9H_{12}$ | 0 |
| 7 | 28.7613% of $C_{12}H_{26}$<br>19.5321% of $C_{14}H_{30}$<br>10.1368% of $\mathbf{C_{16}H_{34}}$ | 19.6855% of $C_7H_{14}$<br>15.6845% of $C_{10}H_{20}$ | 0 | 6.1997% of $C_{10}H_{12}$ |
| 8 | 40.1989% of $C_{12}H_{26}$<br>26.6884% of $\mathbf{C_{16}H_{34}}$ | 14.3968% of $C_7H_{14}$ | 0 | 18.7159% of $C_{11}H_{10}$ |
| 9 | 9.1% of $C_6H_{14}$<br>72.7% of $C_{10}H_{22}$ | 0 | 18.2% of $C_6H_6$ | 0 |
| 10 | 87.0841% of $C_{10}H_{22}$ | 0 | 12.9159% of $C_6H_6$ | 0 |
| 11 | 10.9974% of $\mathbf{C_8H_{18}}$<br>18.3902% of $C_{12}H_{26}$<br>30.2090% of $C_{16}H_{34}$ | 9.7223% of $C_9H_{18}$ | 0 | 30.6811% of $C_{11}H_{10}$ |
| 12 | 28.1328% of $C_{10}H_{22}$<br>19.2691% of $C_{12}H_{26}$<br>15.2804% of $\mathbf{C_{16}H_{34}}$ | 19.7829% of $C_7H_{14}$ | 11.3045% of $C_8H_{10}$ | 6.2303% of $C_{10}H_{12}$ |
| 13 | 18.6725% of $C_{10}H_{22}$<br>38.3681% of $C_{12}H_{26}$ | 26.1542% of $C_{10}H_{20}$ | 16.8052% of $C_6H_6$ | 0 |

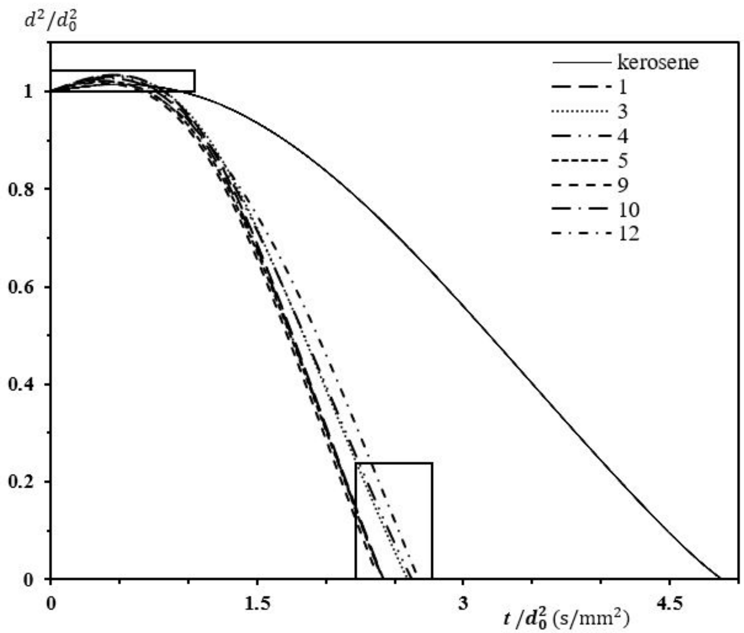
Table 1: Mass fractions of the components of kerosene surrogates (Surr.). 'Ind, Tet & Naph' stands for Indane and Tetraline ($C_{10}H_{12}$) or Naphtalenes ($C_{11}H_{10}$). n-Alkanes are shown in italic, while iso-alkanes are shown in bold.

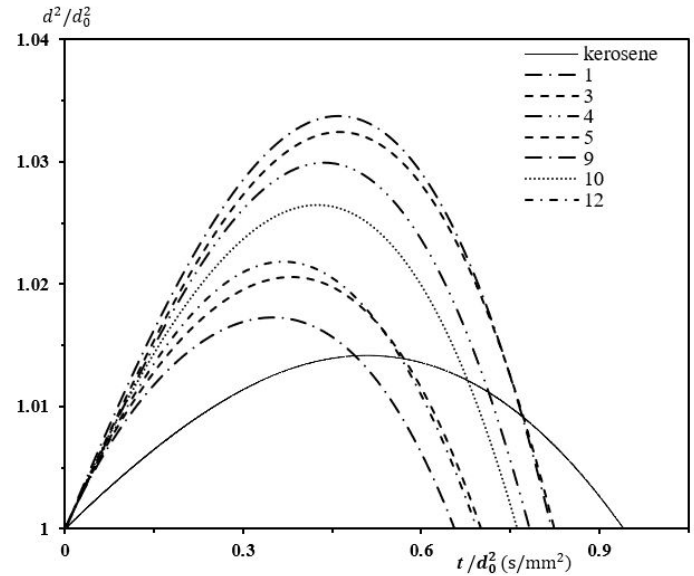
# Surrogate droplets

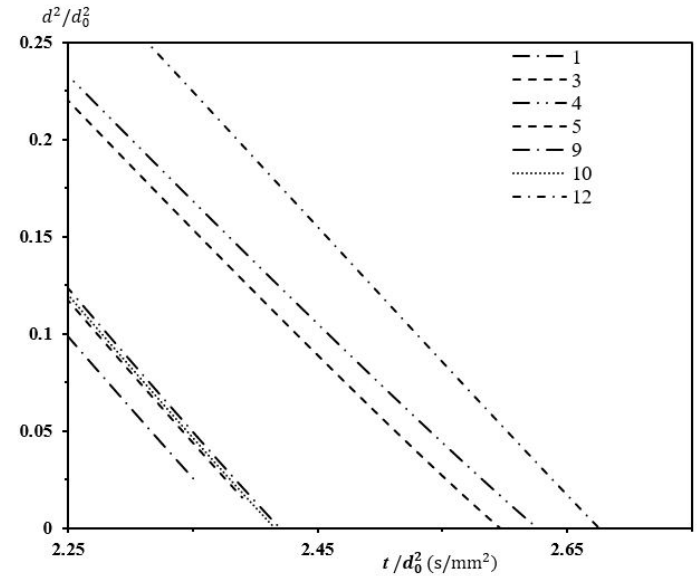
| Surr. | Known as | Refs. |
|---|---|---|
| 1 | Normal decane | [19, 20] |
| 2 | Surrogate C | [21] |
| 3 | Surrogate D | [22] |
| 4 | Surrogate E | [22] |
| 5 | Aachen surrogate | [24] |
| 6 | Modified Aachen surrogate | [22] |
| 7 | Modified Utah surrogate | [25] |
| 8 | Drexel surrogate 2 | [22] |
| 9 | Strelkova surrogate | [26] |
| 10 | Lindstedt surrogate | [31] |
| 11 | Slavinskaya surrogate | [23] |
| 12 | SU1 | O |
| 13 | SU2 | O |

Table 2: Names under which surrogates mentioned in Table 1 are known and the references where they are described. 'O' shows that these surrogates are the original ones developed at Samara National Research University (see Section 2 for further details).

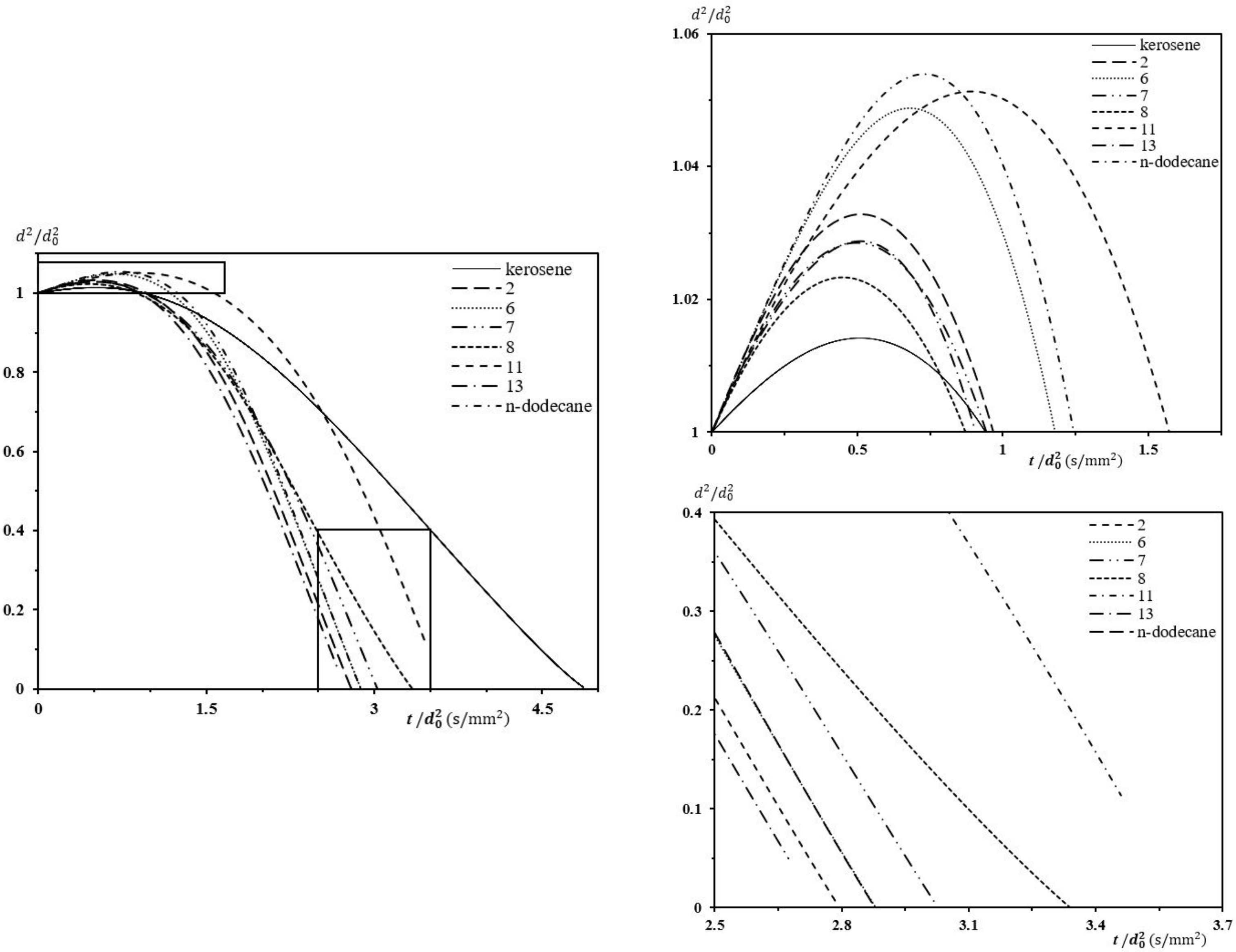
# Surrogate (n-decane dominated)



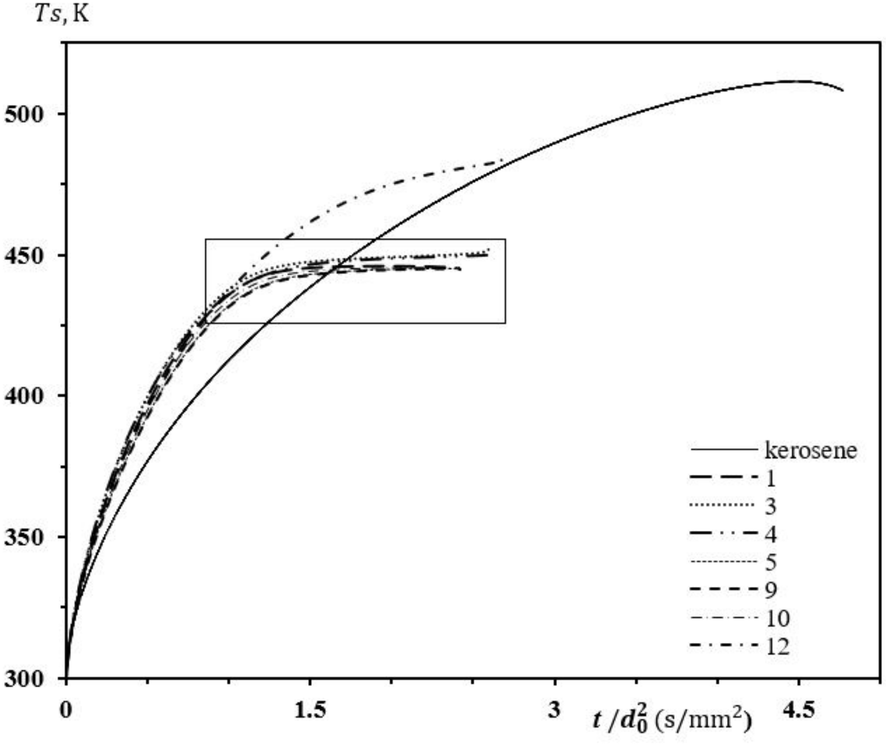



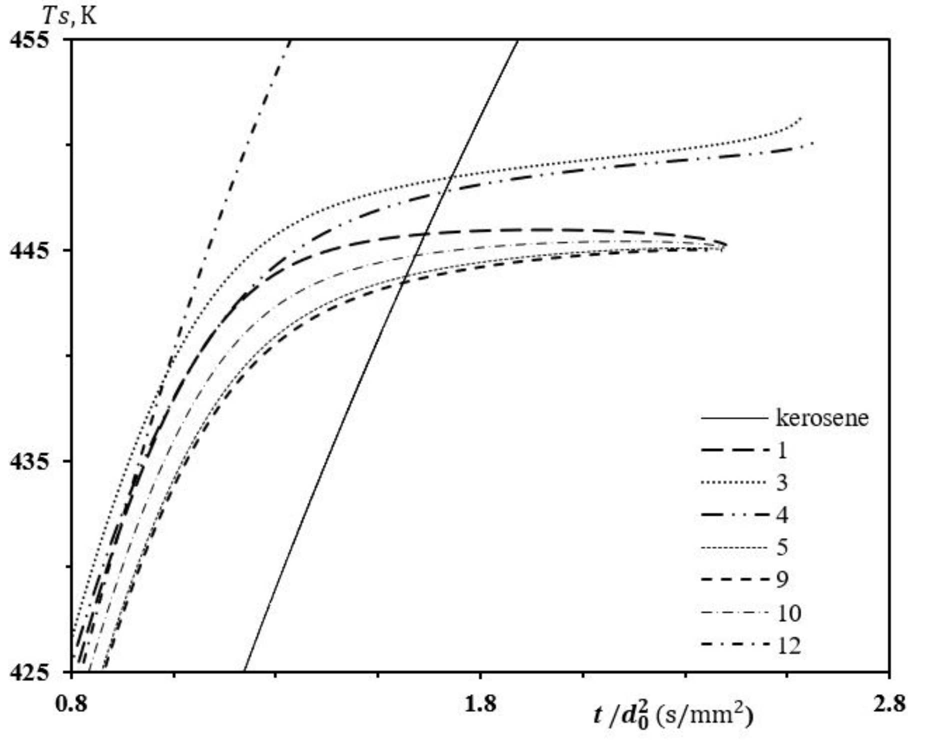



# Surrogate (n-dodecane dominated)

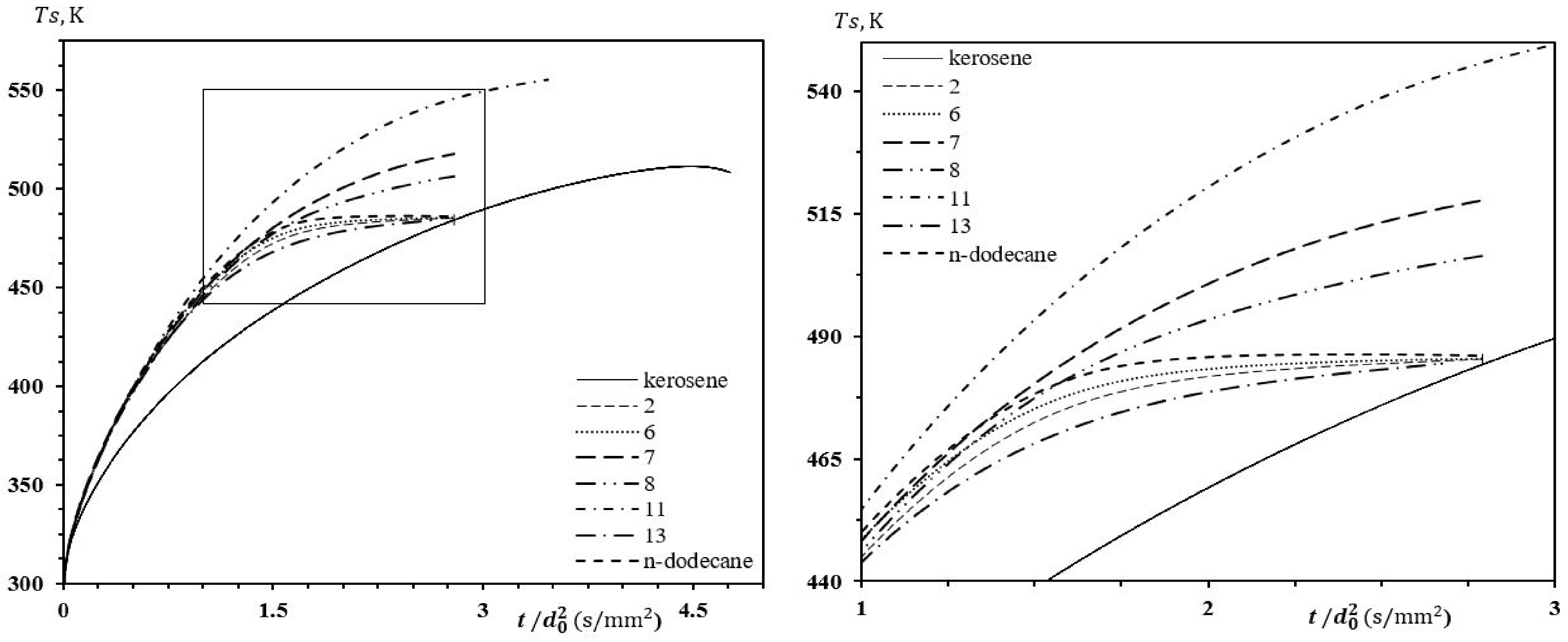


# Surrogate (n-decane dominated)



# Surrogate (n-dodecane dominated)



# Papers

## Evaporation of kerosene droplets: a comparison of the modelling approaches

Luke Poulton[a], Tajwali Khan[b], Oyuna Rybdylova[a,*], Vladimir M. Gun'ko[c], Fang Wang[d,e], Mansour Al Qubeissi[f,g], Sergei S. Sazhin[a]

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[e] *Collaborative Innovation Center of Advanced Aero-Engine, Beijing 100191, China*
[f] *Institute for Future Transport and Cities, Coventry University, Coventry, CV1 5FB, UK*
[g] *School of Mechanical, Aerospace and Automotive Engineering, Faculty of Engineering, Environment and Computing, Coventry University, Coventry, CV1 2JH, UK*

Under review in International J Thermal Science

# Papers

Modelling of surrogate kerosene droplet evaporation: comparative analysis

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[2] *Samara National Research University, 34, Moskovskoye shosse, Samara, 443086, Russia*

In preparation

# Final thoughts

Outstanding issues:

1. Sensitivity of the results to the choice of kerosene composition and approximation of the properties of the components.

2. Surrogates heating, evaporation and autoignition

# Acknowledgements

This work was supported by the UK Engineering and Physical Sciences Research Council [EPSRC Studentship 1792531 and grants EP/M002608/1 and EP/R012024/1]. The UK Fluids network is gratefully acknowledged for its support of the Special Interest Group ‘Sprays in engineering applications: modelling and experimental studies’. This group was a platform for the exchange of ideas between researchers working on various aspects of spray research. This presentation originated in part as a result of this exchange of ideas.

# Thank you for your attention

# Modelling of heating and evaporation of kerosene droplets


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