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Puffing and micro-explosions in composite droplets: recent results

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Abstract
Some of the most recent modelling results concerning the puffing/micro-explosion of water-fuel droplets are summarised. Assuming that the water sub-droplet is located exactly in the centre of the fuel droplet, the component diffusion equation inside the droplets is solved analytically. This analytical solution is incorporated into the numerical code alongside the previously obtained analytical solution for the distribution of temperature inside the droplets. Both solutions are used at each time step of the calculation. The results of investigation of the mutual effects of two and three composite fuel/water droplets, one behind the other, on their puffing/micro-explosion are discussed. The predictions of the model based on the analytical solution to the heat transfer equation in a fuel-water droplet are verified based on their comparison with the predictions of a numerical code for solving the same problem in which this analytical solution is replaced with its numerical solution. The model based on the latter code is generalised to consider a shift of the water sub-droplet away from the centre of the fuel droplet. The models described in the paper do not consider the contributions of the finite time of bubble growth at the start of the puffing/micro-explosion.

Keywords
Nucleation, Composite Droplet, Micro-Explosion, Puffing.

Background

Addition of water into fuel droplets can lead to their puffing (partial disintegration of droplets into relatively large child droplets) and micro-explosion (complete disintegration of these droplets leading to the formation of a cloud of aerosols). Typical images of both processes are shown in Figure 1. The experiments were performed in a heated furnace in which the droplets were supported by a nickel-chromium alloy wire of 0.2 mm diameter as in the experimental setup described in [1]. The initial droplet temperatures were 300 K; the initial droplet radii were about 0.95 mm. The ambient pressure was atmospheric, assumed to be equal to 101325 Pa; the ambient temperature was 850 K.

In our paper and presentation at ICLASS-21 [2] some key results referring to experimental studies and modelling of these processes were briefly summarised. The models for puffing/micro-explosion described in that paper assume that a small spherical water sub-droplet is in the centre of a fuel droplet. The heat conduction equation was solved analytically inside this composite droplet at each time step, using the Robin boundary condition at its surface and the continuity conditions at the fuel-water interface. The Abramzon and Sirignano model [3] was used for the approximation of the droplet evaporation process and the effect of evaporation on the heating process was considered.

The start of puffing/micro-explosion was associated with the time instant when the water/fuel interface temperature reached the water nucleation temperature T_N.

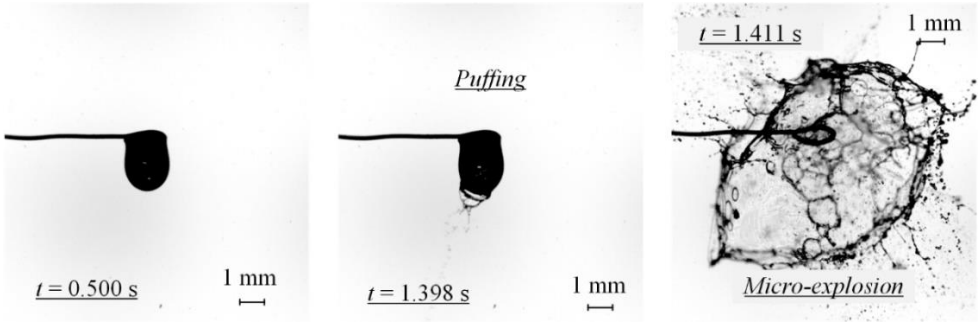

Figure 1. Typical dynamics of puffing/micro-explosion in the experiments performed at National Research Tomsk Polytechnic University (rapseed oil (90%) + water (10%)).

The current paper focuses on the most recent results obtained after publication of [2]. These include modelling of puffing/micro-explosion in multi-component composite droplets, arrays of two and three droplets, and the results of our development of the shift model considering the effects of the shift of the location of water sub-droplet from the centre of the fuel droplet.

Multi-component composite droplets

A model of puffing/micro-explosion of multi-component composite water/fuel droplets, developed in [4], uses the same assumptions as the model described in [2,5] except that the effects of the multi-component nature of the fuel were considered. As in [2,5], it was assumed that a water sub-droplet is in the centre of a spherical fuel droplet. Assuming that the liquid diffusion coefficient is constant for all species at each time step, the component diffusion equation inside the droplets was solved analytically. In this solution it was considered that fuel components do not penetrate into water. Raoult's law was used at the surface of the fuel droplet. The relative diffusion of individual species in the gas phase was not considered. The analytical solution to the component diffusion equation in the liquid phase was incorporated into the numerical code alongside the previously obtained analytical solution for the distribution of temperature inside the droplets. Both solutions were used at each time step of the calculation.

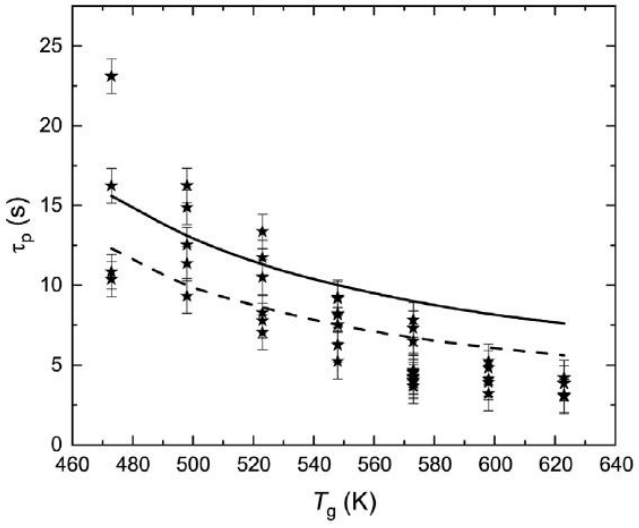

Figure 2. Times to puffing/micro-explosion of water/kerosene droplets (τ_p) versus gas temperatures T_g, observed experimentally (stars) and predicted by the model assuming that puffing/micro-explosion starts when the temperature at the water/kerosene interface becomes equal to the water nucleation temperature ($T_w = T_N$) (curves). The solid (dashed) curve shows the case when the contributions of all kerosene components were considered (kerosene was approximated by cycloundecane). Reprinted from [4], Copyright Elsevier (2022).

The model was used for the analysis of puffing/micro-explosion of kerosene/water composite droplets. The observed times to puffing/micro-explosion τ_p versus gas temperatures are shown in Figure 2. The analysis was focused on kerosene/water composite droplets with initial temperature 300 K, radii 0.85 mm and volumetric water content 10% (R_w=0.395 mm). The experiments were performed at atmospheric pressure. In the same figure, the values of τ_p predicted by the numerical code are presented. It was assumed that puffing and micro-explosion start when the temperature at the water/kerosene interface (T_w) is equal to the water nucleation temperature (T_N). Two cases were considered. Firstly, the contributions of all kerosene components were taken into account. Secondly, kerosene was approximated by cycloundecane and a much simpler model described in [2,5] was used. As can be seen from Figure 2, in both cases the predictions of the numerical code show the same trend of the reduction of τ_p with an increase in ambient gas temperatures. The predictions of the code using both approximations of kerosene are reasonably close to experimental data. The code considering the contributions of all kerosene components predicts longer τ_p than that in which kerosene was approximated by cycloundecane.

Strings of two and three closely spaced droplets

The results of experimental and theoretical investigation of the mutual effects of two and three composite fuel/water droplets, one behind the other, on their puffing/micro-explosion are presented in [6,7]. The case of two closely spaced composite rapeseed oil/water droplets in tandem was considered in [6], while [7] was focused on three Diesel fuel/water droplets. In both cases, the effect of interaction between droplets was considered via modifications to the Nusselt (Nu) and Sherwood (Sh) numbers for these droplets. The focus of [7] was not only on finding the time to puffing/micro-explosion, but also on the investigation of time evolution of temperature at the fuel-water interface before puffing/micro-explosion. The steady state Navier-Stokes equations, the continuity equation for mass, the convection-diffusion equations for the vapour and heat transfers were solved assuming that the droplet arrangement is axisymmetric. Only the normal velocity, corresponding to the Stefan flow, was considered even in the case when Diesel fuel is weakly volatile in the conditions of the experiments. The tangential velocity at the liquid surface was assumed equal to zero.

Both for the cases of two and three droplets it was found that time to puffing/micro-explosion decreases with increasing gas temperature. It was demonstrated that this time for the lead droplet is always shorter than that of the middle (in the case of three droplets) and downstream droplets, and the difference between them decreases as the distance between droplets increases.

Shift model

At pointed out in [8] the model developed in [5] and generalised in several later papers summarised in the previous sections has several important weaknesses. (1) the verification of the model was limited by the development of two separate numerical codes, using Wolfram Mathematica v 12.1 and Matlab R2020a, in which the analytical solution to the heat transfer equation in a composite droplet was implemented. (2) the sensitivity of the results to the shifting of the water sub-droplet location away from the centre of the fuel droplet was not investigated. (3) no quantitative estimates of the effect of this shift on predicted and observed times to puffing/micro-explosion were made. All these three issues were addressed by the authors of [8]. The predictions of the model described in [5] were verified

based on their comparison with the predictions of a numerical code for solving the same heat transfer problem in the fuel-water droplet in which the analytical solution to the heat transfer equation in a fuel-water droplet is replaced with its numerical solution.

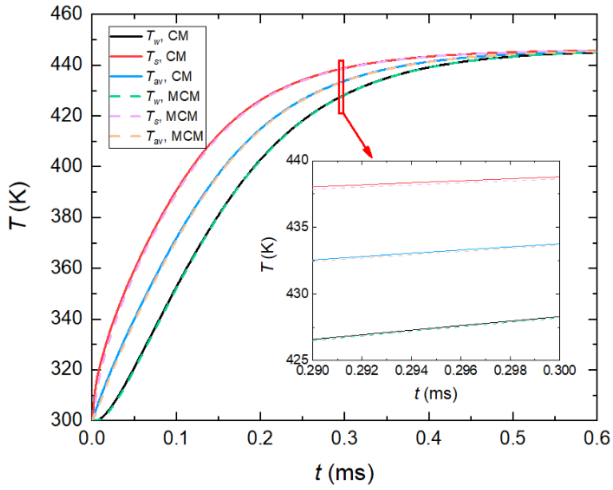

Figure 3. Plots of droplet average (T_{av}) and surface (T_s) temperature and the temperature at the n-dodecane-water interface (T_w) versus time. The curves CM and MCM refer to the results predicted by the model based on the analytical solution to the heat transfer equation in a composite water fuel droplet (Centre Model). The curves MCM refer to the results predicted by the model based on the numetical solution of this equation (Modified Centre Model). Reprinted from [8], Copyright Elsevier (2022).

Plots of n-dodecane droplet average (T_{av}) and surface (T_s) temperatures and the temperature at the fuel-water interface (T_w) versus time, predicted by both codes are shown in Figure 3. The droplet initial radius and temperature were assumed equal to 5 μm and 300 K, respectively. The volume fraction of water was taken equal to 15%. Ambient gas temperature and pressure were taken equal to 700 K and 101325 Pa, respectively. The temperature dependence of the thermodynamic and transport properties of n-dodecane and distilled water were considered [8]. As follows from Figure 3, the results obtained using both models almost coincide. Thus, both models can be considered verified.

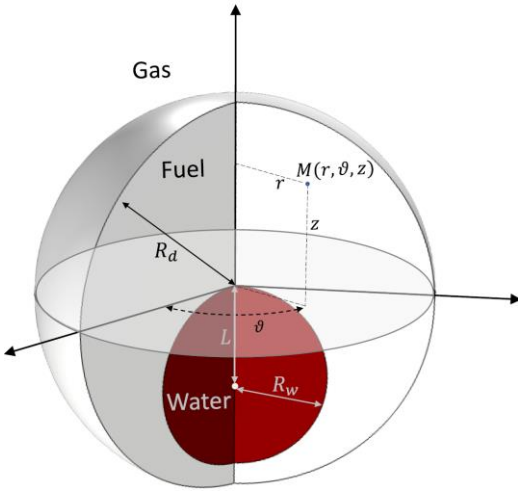

Figure 4. Schematic presentation of the geometry used in the Shift Model. Reprinted from [8], Copyright Elsevier (2022).

The Modified Centre Model (based on the numerical solution of the heat transfer equation in a composite water fuel droplet) was generalised to consider a shift of the water sub-droplet away from the centre of the fuel droplet. This generalisation (hereafter referred to as the Shift Model (SM)) was based on the numerical solution to the heat transfer equation in a fuel-water droplet using the geometry shown in Figure 4. The main simplifying assumption used in the SM is that the surface temperature of the fuel droplet is uniform although it can change with time. Due to the shift in location of the water sub-droplet, a spherical symmetry to the problem was lost. The effect of the shift in the model was described by the normalised shift defined as $S=L/L_{max}$, where L is the distance between the centres of fuel droplet and water sub-droplet (shift), L_{max} is the maximal shift ($L_{max}=R_{d0}-(R_{w0}/2)$), R_{d0} and R_{w0} are the initial values of fuel droplet and water sub-droplet radii, respectively. The values of times to puffing/micro-explosion τ_p for the same input parameters as used for the plots shown in Figure 3 and various S are presented in Figure 5. As follows from this figure, the values of τ_p decrease by less than 1% when S increases from 0 to 0.2. This means that the model developed in [5] can be safely used when S is less than 0.2.

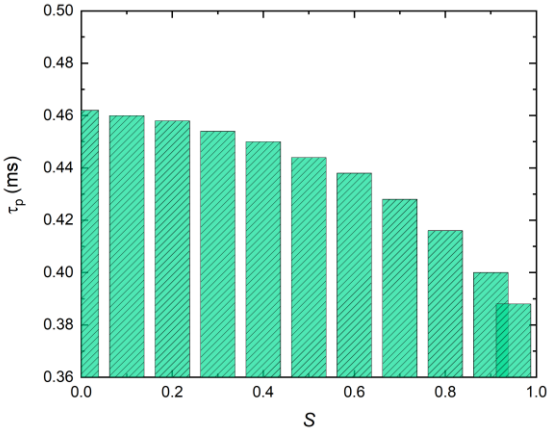

Figure 5. Times to puffing/micro-explosion at various S predicted by the Shift Model for the same parameters as used in Figure 3**.** Reprinted from [1], Copyright Elsevier (2022).

In most cases the values of τ_p predicted by the Shift Model (SM) were shown to be much closer to the experimental data than those predicted by Centre Model.

Summary of other relevant developments

The results of experimental investigation and modelling of puffing/micro-explosion in composite (rapeseed oil mixed with coal micro-particles and water) droplets are described in [9]. The model used in this paper is based on the model described in [5] (Centre Model). Note that the models described so far in this paper do not consider the contribution of bubble growth time to time to puffing/micro-explosion. This effect was considered in [10,11].

Nomenclature

L distance between centres of fuel droplet and water sub-droplet [m]
r radial coordinate [m]
R radius [m]
S normalised shift [-]
T temperature [K]
t time [s]
z axial coordinate [m]

Greek symbols

ϑ azimuthal coordinate [rad]
τ_p time to puffing/micro-explosion [s]

Subscripts
av average
d droplet
g gas
N nucleation
s surface
w water/fuel interface
0 initial

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