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The Effect of Droplet Temperature Model Choice on Gasoline Droplet and Spray Simulation

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Abstract

Prediction of spray droplet temperature is routinely performed within automotive engineering CFD simulation. Important applications include fuel spray modelling for in-cylinder combustion studies and urea-water spray modelling for SCR aftertreatment studies. Transient droplet surface temperature strongly influences droplet and spray evaporation rate and subsequent system performance. In this paper, different droplet temperature models are presented and compared for both single droplet modelling and a single-hole Lagrangian spray CFD simulation in OpenFOAM. The aim is to determine the complexity of implementation of the models and their effect on prediction accuracy for droplet surface temperature, evaporation rate and lifetime. A non-ideal multi-component droplet evaporation model using UNIFAC and NRTL for activity coefficient calculation is used. Model gasoline fuels containing varying quantities of ethanol are studied at conditions appropriate to gasoline direct injection. Three droplet temperature models are compared: a lumped thermal model typically employed in CFD packages; an effective thermal conductivity model (ETC) using the full heat equation; and an ETC model tracking the surface and centre temperature only. For droplet simulations, discrepancies of up to 13% in calculated droplet lifetime are found between the lumped thermal model and the effective conductivity models. The greatest discrepancy in lifetime is observed at conditions and compositions where rapid liquid thermal transients are encountered. This effect is characterized for the first time using the wet-bulb temperature, initial liquid temperature and fuel ethanol content, to guide modellers to an appropriate temperature model for the level of accuracy desired. The effect of droplet temperature modelling in spray CFD simulation is smaller, as measured by maximum changes in spray penetration (2%), evaporation rate (2%) and Sauter Mean Diameter (1.2%). A non-uniform temperature model is required when significant transient temperature change is expected, near-nozzle spray is studied or sub-models such as droplet collision and break-up are not in use.

Introduction

Accurate prediction of gasoline spray behaviour during powertrain multi-dimensional simulations is an important capability for the development of gasoline-fuelled engines. Of particular importance for the development of Gasoline Direct Injection (GDI) engines is the ability to predict and understand the dispersion of fuel within the cylinder; the rate at which it evaporates; and the location of fuel impingement. These influence the subsequent combustion and formation of particulate matter around rich mixture zones, unevaporated fuel droplets or persistent fuel films. Particulate matter emissions from road vehicles, powered by gasoline-fuelled engines, are subject to restrictive legislation worldwide.

Droplet surface temperature has a direct influence on spray evaporation rate because the driving force of evaporation is the fuel saturation pressure at the droplet surface. Therefore, droplet temperature has a controlling influence on droplet and spray penetration, as hotter droplets will tend to evaporate faster, leading to a reduced droplet size and lower penetration of the droplets. It will also influence how quickly droplets align to in-cylinder flows, via control of droplet size. Therefore, accurate prediction of droplet temperatures will have a substantial impact on the prediction of spray shape, structure, and impingement.

The engineering CFD used to model an entire spray, such as a GDI spray, a PFI (Port Fuel Injection) spray or a urea-water spray, typically uses calculations that assume the droplets remain at uniform but time-varying temperature. This is analogous to assuming that the droplets have infinite thermal conductivity, whereby changes to the droplet surface temperature due to interaction with the environment are immediately propagated throughout the entire droplet. This is variously known as a uniform temperature model [1], infinite thermal conductivity (ITC) model [2, 3] and (in this paper) the lumped thermal model. Other approaches can be used to model with greater accuracy the non-uniform temperature distributions that will exist inside the droplets within a gasoline spray. These include the effective thermal conductivity model (ETC) using the heat equation [4, 5]; the effective thermal conductivity model using the two-point model [6]; parabolic temperature distribution and cubic temperature distribution [7]; and analytical solutions [8]. Droplet temperature evolution under flash boiling conditions, using a uniform temperature model, is presented in [9]. A moments-based spray model that calculates a surface area-averaged spray droplets temperature, based on a parabolic temperature profile, is presented in [10]. A review of a number of droplet heating models is available at [3].

Surface temperature prediction is strongly influenced by multicomponent vapour-liquid equilibrium (VLE) and the enthalpy of vaporization (latent heat) of the currently evaporating fraction (not, strictly, the surface composition) [11]. As more volatile components become depleted from the surface via preferential evaporation, the surface temperature may increase or decrease depending on the change in vapour pressure and enthalpy of vaporization. This is particularly important for mixtures containing alcohols, which cause boosted vapour pressure due to their non-ideal mixing with hydrocarbons, but which also have high latent heat [11, 12]. This transient behaviour will also impact the overall droplet temperature via conduction and heat transfer into the droplet interior. The strong

influence of multicomponent VLE has implications for the use of single-component or simplified multi-component mixtures for prediction of fuel spray droplet behaviour.

Adding complexity to the droplet temperature model may add accuracy to the prediction of fuel spray behaviour in a CFD simulation. However, it will also increase the required simulation time. Therefore, this paper provides analysis of the complexity required to adequately predict spray behaviour, under GDI engine, fuel and equipment conditions. This will aid the creation of engine and spray simulations with the best compromise of accuracy and efficiency, to support product development.

In this paper, three droplet temperature models are used in a single droplet evaporation simulation performed in MATLAB and in a spray simulation performed in OpenFOAM CFD. The models considered are the lumped thermal model and the effective thermal conductivity ETC model, implemented with both heat equation and the two-point temperature model. Two multi-component fuels with significant non-ideal behaviour are studied: iso-octane/ethanol and indolene/ethanol using the model indolene fuel from [13]. Both fuels exhibit increasing departure from ideal behaviour when ethanol content is increased. A range of conditions relevant for GDI engine operation is considered in this work: from low pressure, low temperature conditions corresponding to fuel injection during the induction stroke, and higher pressure and temperature conditions corresponding to injection during the compression stroke. Droplet lifetime is reported for the single droplet simulations to compare the effect of model choice, and results are explained via investigation of the transient droplet temperature results. For the spray simulations, overall spray evaporation rate, liquid penetration and overall spray Sauter Mean Diameter are reported. There is only a small change in these metrics when a different temperature model is used. Therefore, further investigation is undertaken to isolate the influence of the temperature model. Local average droplet surface temperature near the spray nozzle shows a significant difference between models, and the influence of temperature model at the whole-spray level is increased when other sub-models are turned off.

Droplet Simulation

Droplet Evaporation Model

Single droplet evaporation simulations were performed in MATLAB, to calculate the droplet lifetime and transient behaviour when different models were chosen for droplet temperature. The evaporation model used is developed from well-established theory [14, 15, 16], representing the evaporation of a single, isolated, spherical droplet, with negligible radiative heat transfer, a quasi-steady gas phase, uniform and constant pressure, and vapour-liquid equilibrium at the droplet surface. A convective enhancement to heat and mass transfer is used to account for rapid droplet motion, relative to the gas phase, encountered in a GDI spray, following [14]. The specific model used in this work is fully described in previous work [1, 11] and further developed here to use the different temperature models presented in this paper. The droplet evaporation rate is given in the model by

$$\dot{m} = \pi \rho_g D \mathrm{Sh`} \ln(1 + B_Y), \qquad \text{Eq. 1}$$

where ρ_g is the fuel vapour/air mixture density; D is the average binary diffusion coefficient of all the fuel species in the ambient gas; Sh` is the modified Sherwood number for convective enhancement, accounting for the blowing effect [14]; and the Spalding mass transfer number B_Y is given by

$$B_Y = \frac{Y_s - Y_\infty}{1 - Y_s}. \qquad \text{Eq. 2}$$

This is calculated from the sum of all fuel species' vapour mass fraction Y at the droplet surface (subscript s) and far from the droplet (subscript ∞). The far-field mass fraction Y_∞ is taken as zero for the single droplet simulations and as equal to the cell total mass fraction scalar for the gas phase in the Lagrangian CFD simulations. The total surface vapour mass fraction can be calculated via the individual fuel species surface vapour mole fractions, given by

$$\tilde{Y}_{s,i} = \frac{\gamma_i \tilde{X}_{s,i} p_{sat,i}}{p}. \qquad \text{Eq. 3}$$

These $\tilde{Y}_{s,i}$ values can be converted to mass fractions, then summed up across all fuel species. Equation 3 is the modified low pressure Raoult's law, with unity fugacity coefficients and activity coefficients γ_i calculated using the UNIFAC method [17] for single droplet simulations and the NRTL method [18] for Lagrangian CFD simulations. The saturation vapour pressure $p_{sat,i}$ of fuel species i is calculated from appropriate correlations recommended in [18], p is the ambient local pressure and $\tilde{X}_{s,i}$ is the liquid surface mole fraction of species i. The well-mixed or batch distillation assumption is employed to allow update of the liquid composition, and uniform internal species composition is assumed. The effect of non-uniform liquid composition on droplet lifetime is explored in [11].

The heating rate Q of the droplets is calculated as [14, 15, 16]

$$Q = \dot{m}\left(\frac{c_{pv}(T_\infty - T_s)}{B_T} - h_{vap}\right), \qquad \text{Eq. 4}$$

where c_{pv} is the fuel vapour heat capacity; T_∞ is the local ambient temperature; T_s is the droplet liquid surface temperature; h_{vap} is the fuel enthalpy of vaporization; and the Spalding heat transfer number B_T is given by

$$B_T = (1 + B_Y)^{\left(\frac{\mathrm{Sh`}}{\mathrm{Nu`\,Le}}\right)}, \qquad \text{Eq. 5}$$

where Nu` is the modified Nusselt number for convective enhancement to heat transfer [14] and Le is the Lewis number, equal to $\lambda_g / \rho_g D c_{pv}$. Here, λ_g is the fuel vapour/air mixture thermal conductivity.

Vapour and liquid phase properties are fully temperature and composition dependent, calculated using guidelines from [18] at $^1/_3$-reference conditions defined as:

$$T_{\mathrm{Ref}} = \frac{2}{3} T_s + \frac{1}{3} T_\infty,$$

$$Y_{\mathrm{Ref}} = \frac{2}{3} Y_s + \frac{1}{3} Y_\infty,$$

Figure 1. Droplet calculation algorithm for ETC full heat equation model

with vaporization enthalpy and vapour heat capacity weighted by currently vaporizing mass fraction [11]. The modified Sherwood and Nusselt numbers are calculated using the Clift *et al.* correlation [19] for the single droplet simulations and the in-built Ranz-Marshall correlation for the Lagrangian CFD simulations (correlation available in [14]).

Lumped Thermal Model

For the uniform temperature model, the rate of change of droplet temperature is given by

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{6Q}{\pi \rho c d^3}, \qquad \text{Eq. 6}$$

where c is the fuel liquid heat capacity and ρ is the fuel liquid density.

Effective Thermal Conductivity (ETC) Model – Full Heat Equation

If the droplet temperature is not constrained to be uniform, the droplet temperature field can be found by solving the liquid heat equation:

$$\frac{\partial T}{\partial t} = \chi \alpha \left(\frac{2}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} \right), \qquad \text{Eq. 7}$$

where α is the droplet thermal diffusivity (variation of which is ignored within the droplet) and χ is the internal vortex enhancement factor originally developed in [4]. This factor takes values in the range 1 – 2.72 depending on the droplet Reynolds number and Prandtl number. The two boundary conditions used in this model at the droplet centre and surface are

$$\left.\frac{\partial T}{\partial r}\right|_{r=0} = 0, \qquad \left.\frac{\partial T}{\partial r}\right|_{r=\frac{d}{2}} = \frac{Q}{\pi \chi \lambda d^2}, \qquad \text{Eq. 8}$$

where λ is the fuel liquid thermal conductivity.

Equation 7 is solved using a finite difference scheme using 5 grid points between droplet centre and surface, which gives satisfactory accuracy with faster results. Recurrence equations for this solution and analysis regarding the errors arising from using this number of grid points is in [1]. A full solution algorithm for the heat equation model is shown in Figure 1.

Effective Thermal Conductivity (ETC) Model – Two-Point Model

This model was developed by Ra and Reitz [6] for implementation in CFD to reduce the number of tracked variables for the Lagrangian phase. In this model, the surface temperature T_s and a representative droplet interior temperature T is tracked. A size-limited surface temperature boundary layer thickness was defined as

$$\delta = \sqrt{\pi \chi \alpha t} \leq \frac{d}{4.514}, \qquad \text{Eq. 8}$$

where t is the current lifetime of the droplet.

In the implementation utilized here, an energy balance is made between droplet heating from the surroundings, the heat required to vaporize the currently vaporizing fuel at the current evaporation rate and droplet heat transferred from liquid surface towards the liquid interior (detailed in [1]). The resulting equation for surface temperature is

$$T_s = \frac{\dot{m} c_{pv} \delta T_\infty + \pi d^2 \chi \lambda B_T T - \delta B_T \dot{m} h_{vap}}{\dot{m} c_{pv} \delta + \pi d^2 \chi \lambda B_T}. \qquad \text{Eq. 9}$$

The droplet interior temperature T can be calculated from Equations 4 and 6, as with the lumped thermal model. This requires an iterative, implicit approach since T_s is a function of $\dot{m}$ which is a function itself of T_s through the surface fuel vapour mass fraction. This model only increases the number of tracked Lagrangian variables by one, instead of adding one for each finite difference gridpoint for the Heat Equation Model.

Spray Simulation

Spray simulations were undertaken using OpenFOAM, version 2.4 [20] for bi-component fuels of iso-octane and ethanol. A Lagrangian Particle Tracking solver was used to model a nominal single-hole plain orifice GDI injector with parameters and model set-up summarized in Table 1. The domain and injection location are shown in Figure 2.

Table 1. OpenFOAM Single-hole GDI Spray Simulation Setup

Parameter	**Value or Option**
Numerical Methods	Lagrangian Particle Tracking, RANS with Standard k-ε turbulence model, PIMPLE algorithm
Domain	30° wedge representing 150 mm length, 80 mm diameter closed chamber
Gas phase	76.6% N_2 by mass, 23.4% O_2 by mass
Injection pressure	150 bar
Nozzle hole diameter	200 µm
Injector cone angle	10°
Injection duration	1.25 ms
Injector flow rate profile	Scaled version from original dieselFoam code [21], giving matched average flow rate to experimental data [22]
Injection method	Rosin-Rammler distribution (SMD = 10 µm, cut off at 30 µm) with prescribed pressure-

	based initial velocity
Primary atomization	Not modelled
Secondary break-up	Reitz-Diwakar model
Collision	Nordin Trajectory model
Turbulent dispersion	Not modelled

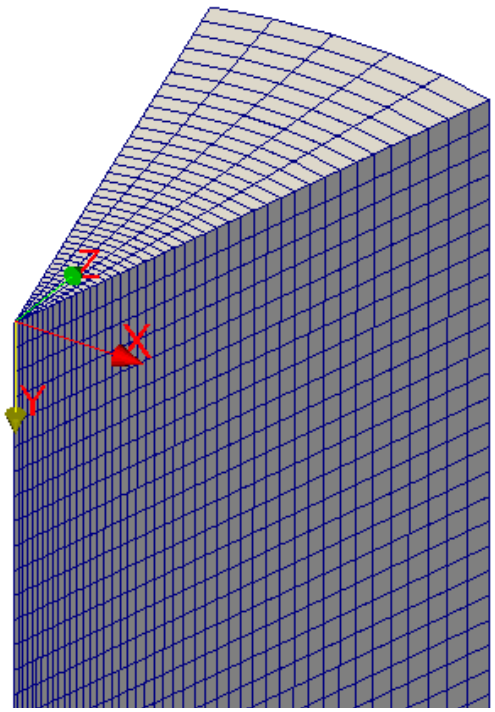


Figure 2. Wireframe view of the spray CFD domain, showing mesh grading, with the injection point at the origin and injection in the positive Y-direction. Periodic boundary conditions are applied to the wedge faces, and wall boundary conditions to the other faces

For droplet temperature modelling, by default OpenFOAM solves Equation 6, using an implicit solution. For comparison, the iterative two-point ETC model was also implemented using Equation 8 and 9. The new surface temperature variable replaced the droplet interior temperature for calculation of enthalpy source terms for solving the gas phase energy equation. The non-ideality of the iso-octane/ethanol mixture was captured in the CFD simulations using the NRTL model for activity coefficients (for Equation 3), using data from [23].

Single Droplet Tests Performed and Results

Single droplet simulations were performed in MATLAB. Droplet velocity was set to 80 m/s, which gives $\chi > 1$, and droplet initial size was set to a representative value of 15 µm. The fuels studied were iso-octane and 8-component indolene, with varying ethanol content by volume, representing current and future EU and US gasoline fuels. The iso-octane/ethanol mixtures and their saturated vapour pressures are shown in Table 2. The composition and saturated vapour pressure of the ethanol/indolene blends are shown in Table 3. The E5, E10, E15 and E20 blends are created by adding 5%, 10%, 15% and 20% ethanol by volume respectively to the E0 blend.

Table 2. Compositions of bicomponent fuel % by volume and calculated indicative saturated vapour pressures at 37.8°C

Component	E0	E5	E10	E15	E20
Ethanol	0	5	10	15	20
Iso-octane	100	95	90	85	80
Calculated vapour pressure (kPa)	11.8	22.1	24.3	24.8	24.6

Table 3. Compositions of ethanol-indolene fuel % by volume and calculated indicative saturated vapour pressures at 37.8°C

Component	E0	E5	E10	E15	E20
Ethanol	0	5.00	10.00	15.00	20.00
n-Butane	6.09	5.78	5.48	5.18	4.87
Iso-pentane	16.13	15.32	14.51	13.71	12.90
Cyclohexane	18.27	17.35	16.44	15.53	14.61
Iso-octane	16.22	15.41	14.60	13.79	12.97
Toluene	15.81	15.02	14.23	13.44	12.65
Ethylbenzene	12.68	12.04	11.41	10.77	10.14
n-Decane	12.46	11.84	11.21	10.59	9.97
Naphthalene	2.35	2.23	2.12	2.00	1.88
Calculated vapour pressure (kPa)	61.7	68.9	69.0	68.3	67.5

Simulations were performed at a range of initial droplet temperatures (injection temperature) T_0, and ambient temperatures T_∞ and pressures p, using E5-E20 mixtures for iso-octane/ethanol and E0-E20 mixtures for indolene/ethanol. The range of conditions considered are shown in Table 4 for iso-octane/ethanol and Table 5 for indolene/ethanol, along with the results for life-time discrepancies between the temperature modelling approaches. The lumped thermal model and the two-point ETC model are compared with the full heat equation ETC model, and the fuel composition with the highest life-time discrepancy is reported.

Table 4. Iso-octane/ethanol single droplet simulation results, with fuel composition giving the greatest discrepancy between modelling approaches. A positive discrepancy means that the lumped thermal model gives a longer droplet lifetime

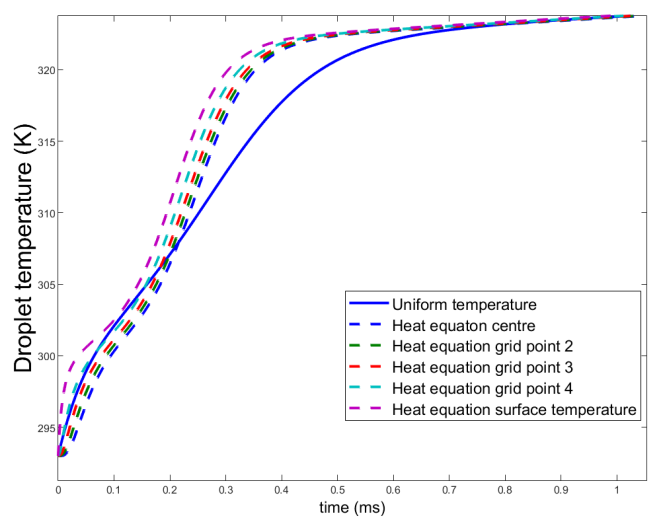
			Lumped vs Heat Equation		**Two-point vs Heat Equation**	
p (bar)	T_0 (K)	T_∞ (K)	Fuel	% lifetime discrepancy	Fuel	% lifetime discrepancy
0.5	293	293	E5	-4.5	E20	-0.1
		373	E10	-3.9	E10	0.9

		453	E10	-1.7	E10	1.3
1	293	293	E5	-3.3	E10	0.1
		373	E15	-2.1	E10	0.9
		453	E5	6.3	E20	1.3
3	293	453	E5	8.3	E5	2.2
		573	E5	10	E15	0.7
	363	453	E20	-8.1	E5	0.3
		573	E5	2.4	E15	-1.8
6	293	453	E5	8.4	E5	0.7
		573	E5	13.2	E15	0.7
	363	453	E20	-5.5	E15	0.8
		573	E5	6.4	E10	1.4
	393	453	E20	-13.1	E20	-1.8
		573	E5	-4.9	E20	-1.4

Table 5. Indolene/ethanol single droplet simulation results, with fuel composition giving the greatest discrepancy between modelling approaches. A positive discrepancy means that the lumped thermal model gives a longer droplet lifetime

			Lumped vs Heat Equation		**Two-point vs Heat Equation**	
p (bar)	T_0 (K)	T_∞ (K)	Fuel	% lifetime discrepancy	Fuel	% lifetime discrepancy
0.5	293	293	E20	-0.7	E20	0
		373	E15	-2	E0	0.4
		453	E0	1.6	E15	0.7
1	293	373	E10	-0.9	E0	0.5
		453	E0	2.7	E0	0.8
3	293	453	E0	5.2	E0	1
		573	E0	10.1	E15	1.1
	353	453	E0	-7.1	E5	-0.7
		573	E5	-4.7	E0	-0.4
6	293	453	E0	6	E15	1
		573	E0	12	E0	1.2
	353	453	E20	-4.5	E10	0.3
		573	E10	-2.1	E0	1.1
	383	453	E0	-10.1	E0	-0.5
		573	E20	-6.7	E0	-1.2

There is significant inaccuracy from using the uniform temperature lumped thermal model at some conditions and fuel compositions. This occurs for both the bicomponent and the multi-component fuels tested. This is attributed to conditions at which there is a large transient in the droplet's temperature. Droplets will either cool down or heat up towards the wet-bulb temperature of the initial composition: if this wet-bulb temperature is quite different from the initial droplet temperature T_0 (representing the injection temperature), there will be a large transient. For example, there was observed a large transient droplet temperature increase for ambient conditions of 1 bar, 453 K and initial droplet temperature of 293 K, whereas there was a large cooling transient for the droplets at initial temperatures 393 K in the same ambient gas conditions. The effect this has on droplet lifetime is illustrated in Figure 3. Initially, as expected, the lumped thermal model temperature follows an intermediate temperature compared to the surface and centre temperatures predicted from the heat equation. However, it is the surface temperature that controls the evaporation rate. Therefore, in this case, the heat equation model predicts a faster evaporation rate due to the higher surface temperature. The most volatile species here is ethanol and under a slightly increased temperature it will evaporate relatively faster from the droplet than iso-octane. This is shown in the ethanol composition (mole fraction) history in Figure 3, where under the heat equation model the ethanol is more rapidly depleted. There is a rapid fall off in mixture non-ideality, and hence mixture vapour pressure, as ethanol content reduces (see Table 2). Thus, the droplet modelled with the heat equation becomes less volatile, meaning less heat is used to create vapour and a greater proportion gives rise to heating of the droplet. (There is not a significant effect via reduction in enthalpy of vaporization as ethanol content is reduced, because it the enthalpy of vaporization of the currently vaporizing fraction that features in Equation 4.) This causes the temperature history of the two models to further diverge, only to reunite after all the ethanol has evaporated as both converge towards the pure iso-octane wet-bulb temperature for these conditions. Therefore, the heat equation model has a significant period of higher temperature, resulting in a faster overall evaporation and shorter droplet lifetime at this condition.



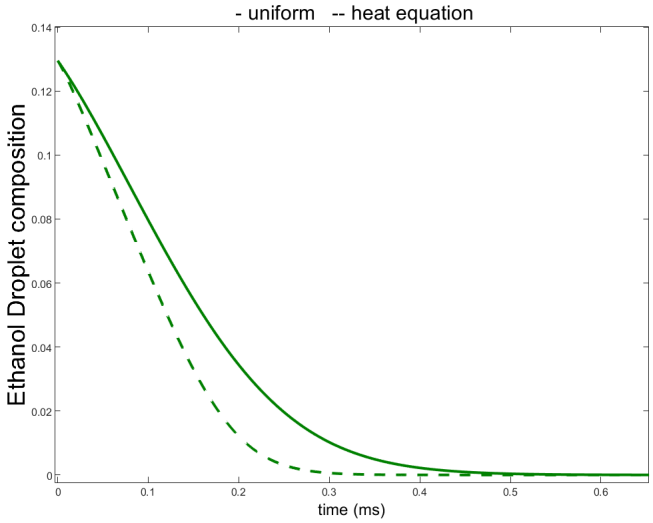


Figure 3. Transient temperature discrepancy *(top)* and composition (mole fraction) discrepancy *(bottom),* between the heat equation model and the lumped thermal model, for the case of E5 iso-octane/ethanol mixture at 1 bar, 453 K ambient conditions with initial droplet temperature of 293 K

A means was sought of predicting whether there would be a significant droplet temperature transient that would cause the simpler lumped thermal model to be in error. Two main factors were thought to cause this for the GDI fuel droplet studied here: the magnitude of the transient temperature change and the quantity of ethanol present in the droplet. Fuel mixtures with greater ethanol content will retain ethanol in the droplet for a longer proportion of the droplet lifetime, under the well-mixed/batch distillation model, leading to lower surface temperatures and a tendency for evaporation rate underprediction. This means that there will be a longer period of surface temperature discrepancy between the models, before return to the temperatures predicted for pure hydrocarbons, as shown in Figure 3.

For each of the fuels and conditions studied, the wet-bulb temperature T_{WB} was calculated. A suitable metric for indicating whether the lumped thermal model will cause an error was found by calculating $T_{\mathrm{WB}} - T_0 - kE$, where E is the percentage by volume content of ethanol in the fuel. A useful result was found by setting $k = 1$, as shown in Figure 4. As can be seen, a positive value of $T_{\mathrm{WB}} - T_0 - kE$ indicates that the ETC model predicts a faster evaporation. For large negative values of $T_{\mathrm{WB}} - T_0 - kE$, the lumped thermal model predicts a faster evaporation. For values of $T_{\mathrm{WB}} - T_0 - kE$ between -40 K and 0 K, this approach advises that the predicted lifetime discrepancy will be lower than 5% and that the lumped thermal model will provide a good description of the droplet behaviour.

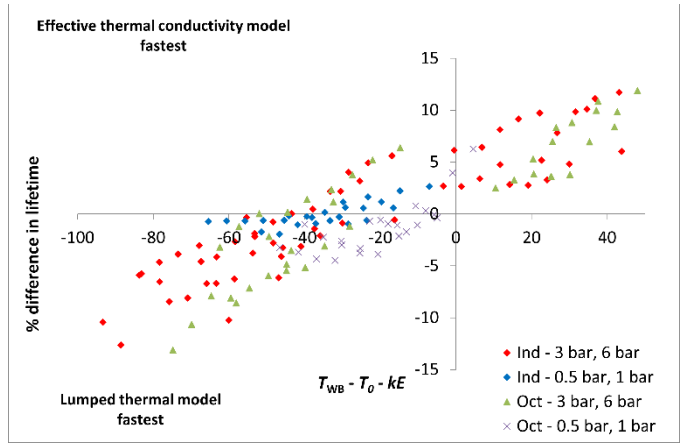


Figure 4. Plot of $T_{\mathrm{WB}} - T_0 - kE$ for each of the single droplets studied versus the lifetime discrepancy between the lumped thermal model and the full heat equation ETC model. The parameter $k = 1$. Data points marked Ind are indolene/ethanol mixtures and marked Oct are iso-octane /ethanol mixtures

The two-point model and the heat equation model are in close agreement for droplet lifetime predictions, with the maximum discrepancy of 2.2% for the bicomponent fuel at ambient conditions of 3 bar and 453 K with an initial liquid temperature at 293 K for the E5 fuel. The average absolute difference between the models was 0.5% for the low pressure (0.5 bar and 1 bar) cases collectively, which is comparable to the inaccuracies found in the heat equation grid sensitivity study in [1]. Discrepancies between these two models were magnified at the high pressure cases, representing fuel injection during the compression stroke (3 bar and 6 bar), with an average absolute difference between the predicted droplet lifetimes of 1.6% for the bicomponent fuel and 0.7% for the multi-component indolene fuel. This is due to the higher transient temperature change during the early part of the droplet life that was observed in these cases.

The computational run time for a single droplet simulation using the two ETC models in MATLAB was compared. The two-point model had an average run time of 88 seconds. The heat equation model, with only 5 grid points, had an average run time of 107 seconds. This indicates that the two-point model is likely to be fastest, though it should be noted that efficiency of implementation into a commercial code (based on, for example, C++ or FORTRAN) may affect this comparison.

Spray Tests Performed and Results

Following the single droplet simulations, whole spray tests were performed in OpenFOAM, using iso-octane/ethanol fuel mixtures. Conditions were chosen that exhibited the largest differences in single droplet lifetime prediction due to temperature model choice, to determine how this observation applied to a full gasoline spray. The chosen test points are shown in Table 6.

Table 6. Test Cases for Spray CFD temperature modelling comparison. A positive discrepancy means that the lumped thermal model gives a longer droplet lifetime

Case	p (bar)	T_∞ (K)	T_0 (K)	Ethanol content by volume	Single droplet lifetime discrepancy

1	1	293	293	E5	-3.3
2	1	453	293	E5	6.3
3	6	573	293	E5	13.2
4	6	453	393	E20	-13.1

Figure 5 shows the on-axis average droplet surface temperature histograms for the spray, binned into 5 mm intervals for the four cases outlined in Table 6, gathered at the end of injection. For the lumped thermal model, the surface temperature is the same temperature as the rest of the droplet, whereas in the two-point model the surface temperature is explicitly modelled and tracked for each Lagrangian parcel using Equation 9. These results show in each case that there is a faster transient response in droplet temperature predicted from the two-point model: in Cases 1 and 4, droplets reach colder temperatures more quickly and in Cases 2 and 3, droplets reach hotter temperatures more quickly. This mirrors the findings from the single droplet tests. However, the discrepancy in surface droplet temperature has become insignificant within 20 – 40 mm from the injector.

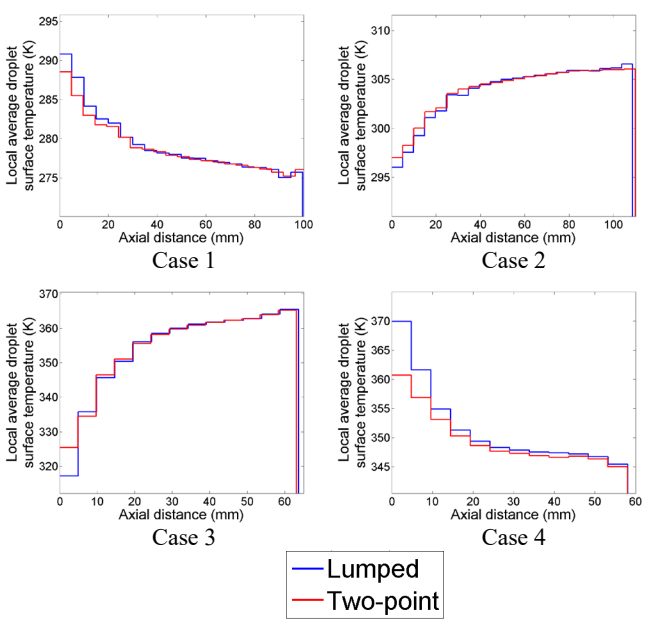


Figure 5. On-axis averaged droplet surface temperature for each spray CFD case from the two temperature models implemented: the lumped thermal model and the two-point model

The spray-wide average SMD is shown in Figure 6 for Case 1 and 2. This figure shows that the effect of the temperature model in the spray simulation is slight, once the spray has begun. For Case 1, it was expected from the single droplet simulations that the lumped thermal model would overpredict evaporation rate: the lumped thermal model resulted in an end of injection SMD lower by 0.03 µm for Case 1. For Case 2, it was expected that the lumped thermal model would underpredict evaporation rate: the two models alternated between largest SMD value, with the lumped thermal model resulting in the smallest SMD at the end of the simulation. In addition, there was a small change in overall spray mass evaporation rate until the end of injection, which is 2% reduction for Case 1 but a negligible change for Case 2. A 1.5% change in liquid penetration was observed for both cases at the time of end of injection (using a 95% liquid mass threshold). This was an increase in penetration for Case 1 due to the presence of more, larger, slowly evaporating droplets that reach colder temperatures faster; and a decrease in penetration for Case 2 due to the presence of more, smaller, faster evaporating droplets that reach hotter temperatures faster.

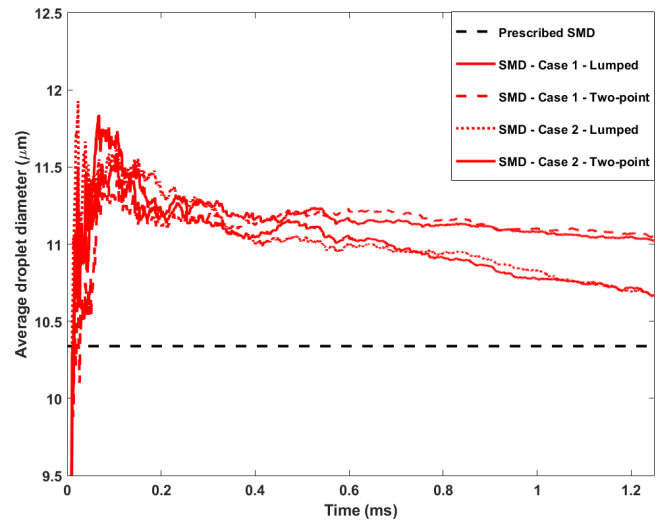


Figure 6. Spray-wide SMD for Case 1 and 2. The time period shown is the duration of the injection

It was hypothesized that this more marginal response to the change in droplet temperature model with the full spray simulation compared to the single droplet simulation could be attributed to several factors. Firstly, the gas phase coupling in the Lagrangian spray simulation means that the spray vapour and gas that droplets pass through are significantly closer to the spray droplets' temperature than was the ambient gas to single droplets' temperature in the MATLAB simulations. Secondly, droplet collision (specifically the coalescence scenario) and secondary break-up modelling, which are typical in spray modelling, cause a reset in the droplet to a uniform temperature distribution. As there was no meaningful way to apportion surface temperature and interior temperature to child droplets of break-up events or to transfer surface and interior temperature to a newly formed droplet coalescence, no means was attempted in this work. This meant that coalescence or break-up events disrupted and reset the divergence of temperature histories observed between the lumped thermal model and the two-point model in the single droplet simulations. To assess the effect of this, Case 2 was rerun without break-up or collision, and then further with no gas phase coupling, with the results shown in Figure 7. Both runs now show the lumped thermal model with the largest SMD throughout the injection duration. Increasing divergence is observed between the SMD obtained with the lumped thermal model and with the two-point model, as more of the other spray simulation features are removed, to return the droplets towards isolated droplet evaporation studies. With no break-up or collision, the lumped thermal model SMD is 0.02 µm larger than the two-point model at 1.25 ms; with gas phase coupling, it becomes 0.11 µm larger at 1.25 ms.

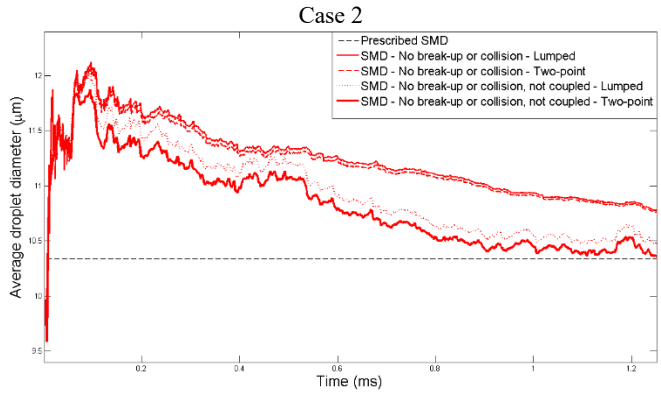


Figure 7. Case 2 SMD across the spray, with rerun simulations: firstly, with collision and break-up sub-models turned off; secondly, with gas phase coupling turned off as well

Cases 3 and 4 both had a larger initial temperature difference between gas and liquid, which meant that there was a larger transient of significant temperature difference between droplet and surroundings, which in turn drove differing behaviour under the two droplet temperature models. Thus, as can be seen in Figure 8, there is a greater difference in overall spray mass evaporated for both Case 3 and 4: at end of injection there is a difference of 0.7% of injected mass for Case 3 and 1.3% of injected mass for Case 4. This is combined with a 2% difference in liquid penetration for Case 3 and negligible for Case 4

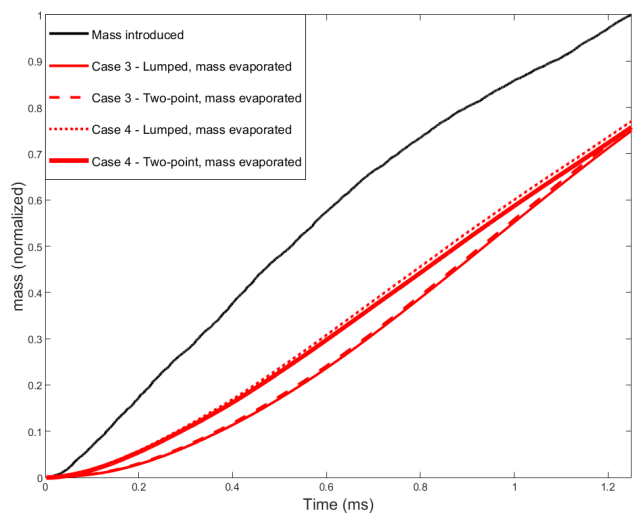


Figure 8. Case 3 and Case 4 spray masses. Mass injected *(black)* and mass evaporated *(red)*

Conclusions

Models for droplet heating have been investigated, using both single droplet simulations and full spray CFD simulations, to compare a lumped thermal model as typically employed in CFD with two effective thermal conductivity models (ETC). The ETC models were implemented using a two-point temperature model and a full heat equation model. Ethanol-containing model gasoline fuels were used to represent current and future gasoline blends, with the strong non-ideal behaviour of ethanol/hydrocarbon mixtures accounted for by activity coefficient models. A range of conditions were used to evaluate the relative performance of these models, which were representative of gasoline direction injection during either the induction stroke or the compression stroke.

The lumped thermal model kept a uniform temperature throughout the droplet lifetime and gave adequate single droplet lifetime predictions as well as temperature and composition history at lower ambient temperature conditions, corresponding to early injection strategies.

However, the lumped thermal model predicted up to a 13% longer or shorter lifetime than the heat equation model at conditions where large temperature transients were expected, either heating or cooling. The source of error is caused by incorrect prediction of surface temperature and hence evaporation rate, exacerbated by highly non-ideal mixtures such as ethanol/iso-octane. To predict when the more complex ETC model would be needed, the parameter $T_{\mathrm{WB}} - T_0 - kE$ can be evaluated for the given fuel composition, initial fuel temperature and ambient conditions. In this paper, with $k = 1$, it is shown that values of $T_{\mathrm{WB}} - T_0 - kE$ outside of the range -40 K to 0 K will result in a greater than 5% lifetime discrepancy when the simplest lumped thermal model (uniform temperature) is used.

The two-point model and the heat equation model were at most different by 3.3% in droplet lifetime prediction, and usually much closer. Following a previous study into grid size dependency for the heat equation model, it is anticipated that the predictions from the two-point model are at least as accurate as those from the heat equation model using a small number of grid points. In this study, even with only five grid points, the heat equation model was slower to execute than the two-point model by 20%. Therefore, at conditions where it is necessary to use an ETC model, such as when a large transient droplet temperature change is expected, it is recommended to use the two-point model in both droplet simulations and spray CFD.

Simulations of a simple single hole gasoline spray, at realistic GDI engine conditions, have been performed in OpenFOAM to demonstrate the application of a non-uniform droplet temperature model (two-point model) to a full spray, in comparison to the lumped thermal model. The different responses of the four spray cases studied in this paper, in terms of spray penetration, evaporation rate and SMD, shows that the effect of temperature model choice does not immediately follow from findings from single droplet studies. At low temperatures, representing induction stroke injection, there was only a minor effect of temperature model choice – with less than 2% change in evaporated spray mass and spray liquid penetration observed, and <1% change in spray overall SMD. The change in temperature model, and discrepancy in droplet temperatures, was dominated by the coalescence and break-up of droplets and by the gas phase coupling, which greatly reduced the local ambient temperature in which the spray droplets exist. At higher temperature conditions, the same trends as seen for single droplets were seen in the spray, which resulted in noticeable changes to mean droplet sizes (up to 1.2% in spray SMD), mass evaporated (1.7%) and liquid penetration between models (up to 2%). In conclusion, the use of the more computationally intense two-point temperature model, or similar temperature model, is only recommended for GDI sprays when there is significant transient temperature changes or if accurate prediction of the near nozzle spray is the target of the simulation exercise.

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