Prediction of the hydrodynamic characteristics of 2,5-dimethylfuran fuel sprays using the moments of the droplet size distribution

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Abstract

The moments-based spray model has been developed as an alternative to the widely used discrete droplet models; the model does not characterize sprays using droplet size classes, rather the moments of the droplet size distribution are used. 2, 5-Dimethylfuran (DMF) has been receiving some interest of late as a potential gasoline-like biofuel. Compared to bio-ethanol, DMF is attractive because the gravimetric energy density is higher, it is easier to store, less volatile, and easier to transport. In the present study, the moments-based spray model has been used to predict the hydrodynamic properties of DMF fuel sprays.

The results of the evaluation of DMF fuel sprays at 50 bar injection pressure and different ambient (1 to 6 bar) pressure values are presented, evaluated and compared with experimental data. The results are characterized by the fuel spray penetration values at the end of injection and at various times after the start of injection. This information is important for the design of injection and combustion systems in internal combustion engines, especially as fuel spray impingement on walls can lead to increased emissions. The results indicate that DMF fuel spray penetration reduces with increases in ambient pressure as the fuel droplets are slowed due to the increased frictional resistance offered by the carrier gas. The predicted results for the fuel spray tip penetration at the end of injection are representative of the measured experimental fuel spray development. The predictions are also compared with results from a spray model based on the widely used discrete droplet method. The results show that the moments-spray model can be a valuable tool for evaluating the characteristics of emerging biofuel sprays.

Keywords

Moments-spray model, dimethylfuran, discrete droplet method, spray penetration, droplet size distribution.

Introduction

As concerns over the availability and non-renewable nature of fossil fuels continue, alternative fuels, including biofuels, are being explored. However, for any alternative fuel to be a viable alternative to current fossil fuels, it must have thermo-physical properties that have made current non-renewable fuels attractive in terms of energy density, storage, operating conditions and ease of production. Ethanol fuel, which can be produced from biomass such as grain and sugarcane, is the main biofuel currently available in large quantities, with worldwide production in 2015 estimated at over 25,600 million gallons [1]. However, Ethanol fuels can hydrate and have about 67% gasoline gallon equivalent (energy content of gasoline) [2].

2, 5-dimethylfuran (DMF) has several advantages compared to Ethanol. It has a higher energy density (by up to 40%, like that of gasoline), does not hydrate [3], and improved production techniques have been presented [3, 4].

Thus, DMF has attracted the attention of internal combustion engine researchers. Zhong *et al*. [5] compared results from using DMF in a research engine with data from gasoline and ethanol fuelled engines and the results showed that the combustion performance and the emissions where not dissimilar to those of commercial gasoline. Tian *et al* [6] studied the spray characteristics of DMF and blends of DMF fuel sprays. The results indicated that the droplet sizes of the DMF fuel spray and its blends were smaller than those of the ethanol fuel spray, and they decreased in size faster than those of the ethanol spray as the fuel injection pressure is increased. It appeared from the studies that the characteristics of the DMF fuel spray are more fitting to a gasoline engine than those of ethanol fuel sprays, as was also the case with studies from Daniel *et al* [7].

Few numerical simulation studies of the characteristics of DMF fuel sprays exist. Li *et al* [8] modelled the primary and secondary atomization stages of DMF fuel sprays using the KIVA 3V code and the results indicated that significant spray-wall splashes, and inadequate mixing time add to the poor air/fuel distribution seen in the DMF fuel spray compared to the more homogeneous gasoline fuel spray mixture.

Typically, computational fuel spray models are based on the discrete droplet model, in which the turbulent carrier gas equations of motion are solved in an Eulerian scheme, and the liquid droplets equations of motion are solved using a Lagrangian scheme. The approach has been successful as groups of identical droplets can be efficiently described in the liquid phase and it is easier to represent the dispersed liquid phase in a Lagrangian manner. However, a large of number of groups of identical droplets must be tracked with this method to allow a representative sample of droplets resulting in computational expense.

In an alternative to the discrete droplet model the carrier gas and liquid phases are modelled using an Eulerian scheme and the first four moments of the droplet-size-number distribution are used to describe the full polydisperse nature of the fuel spray. Several variations of the moments-method model have been presented. In [9 – 14] the last three moments of the droplet-size-number distribution function are calculated from transport equations, whilst the first moment is evaluated from a general Gamma distribution function. In [15] the four moments of the droplet-size-number distribution function are evaluated from transport equations and the method applied to diesel fuel spray cases. In [16 - 18] the last two moments of the droplet-size-number distribution function are evaluated from transport equations and the first two are approximated from a presumed droplet number size distribution. The 'three-moment' model [9, 10] has been used for the numerical studies of DMF fuel sprays presented in this paper. This is mainly because it is computationally less intensive than the 'four-moment' model [15] largely because three transport equations are solved for the moments of the droplet-size-number distribution function rather than four, and less assumptions are made with respect to the derivation of the droplet-size-number distribution function compared to the 'two-moments' model [17, 18]. In this study DMF fuel sprays are evaluated at different ambient pressure values. The spray structures and the fuel spray tip penetration values are evaluated and compared to results from experimental data and from a discrete droplet model.

The rest of the paper describes the numerical modelling used, the nature of the experiments used for the assessment and the evaluation of the results from the model.

Mathematical models

Droplet size distributions

If a volume distribution function is proportional to the droplet number distribution function $n(r)$, which represents the distribution of a number of droplets over a range of droplet diameters, and this function is integrated over all droplets and weighted, the total number of droplets can be described as:

$$Q_0 = \int_0^\infty n(r)dr \tag{1}$$

The *i* th moment of this distribution can be written as:

$$Q_i = \int_0^\infty n(r)r^i dr \tag{2}$$

The second moment Q_1 represents the total sum of drop radii, per unit total volume, the third moment can be presented in terms of the surface area of the drops per unit total volume as $4\pi Q_2$, whilst the fourth moment can defined in terms of the liquid volume per unit total volume $4\pi Q_3/3$

The moments defined in equation (2), Q_0, to Q_3, contain a lot of information about the spray and therefore can be used to represent fuel spray characteristics by using representative diameters such as the Sauter Mean Diameter:

$$D_{32} = \frac{Q_3}{Q_2} \tag{3}$$

Moment Transport Equations

For the work presented here, the first moment Q_0, is calculated from a Gamma number distribution and the last three moments Q_1, Q_2 and Q_3 are evaluated by means of transport equations. From [9, 10] the set of the moment transport equations can be presented in this form:

$$\frac{\partial Q_i}{\partial t} + \frac{\partial}{\partial x_j}(Q_i U_{lij}) = -S_{Q_i} \tag{4}$$

Equation (4) presents the moment-average velocity U which provides the method that enables the distribution of the droplet sizes to vary in space and time. S_{Qi} represent the effects on the moments of drop break-up, drop collisions and evaporation. The effects of droplet evaporation are not considered here but have been presented previously [13], and the complete presentation of the droplet breakup dynamics in [10].

Thus, the complete representation of the nature of the polydisperse spray is possible in the moments-method through:

- The definition of the droplet number moments. This provides the droplet size distribution at each point in space and time,
- The definition of the moment-averaged velocities. This provides how the droplet size distribution changes in space and time, and
- The combination of the two concepts above.

Discretization and Solution methods

All the transport equations and the droplet moment equation (equation (4)) are discretized using a finite volume scheme. The equations are solved on a two-dimensional, axisymmetric, orthogonal computational grid (Figure (1)) using an Eulerian scheme, and a k - ε turbulence model since the carrier gas is considered turbulent. An Euler implicit method is used for the temporal differencing and the spatial differencing is done using a hybrid scheme which involves a second-order-accurate central differencing scheme for the computational cells with low Reynolds numbers and a first-order upwind scheme for computational cells with high Reynolds numbers [9, 16]. This aids the stability of the schemes.

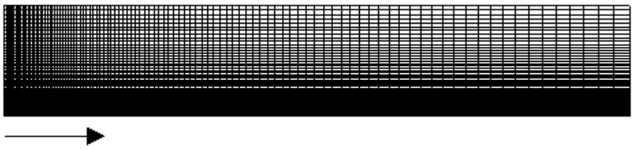

Figure 1. Grid used for the numerical solutions. The domain is 200 mm x 37 mm. The injector is located on the bottom left hand side, and sprays across the centerline to the right.

Experimental Data

The experimental data used for this work were derived from the work of Li [20]. A shadowgraph system consisting of a Charge Coupled Device (CCD) camera, a lamp system, an injector with the tip connected to a constant volume vessel and driven by a pump were used. The injection pressure and duration were set at 50 bar and 2 ms respectively. The ambient pressure was set at 1, 3, and 6 bar by varying the pressure gauge connected to the vessel. The spray image, illuminated by the lamp, was captured by the CCD camera. The DMF fuel was injected at 20 °C room temperature into an open environment which is like the conditions of a gasoline direct injection (GDI) engine at early injection. Experimental data for DMF fuel spray tip penetration at the 3 ambient pressure cases were given. Some properties of the DMF fuel used for the experiments are presented in Table (1).

Table 1. Properties of DMF fuel used by Li [20].

Fuel property	2, 5 Dimethylfuran (DMF)
Molecular Mass	96.13 g mol^{-1}
Density @ 20 °C	895.4 kg m^{-3}
Surface Tension	25.9 dyne cm^{-1}
Viscosity @ 20 °C	0.65 cP

Numerical Parameters

The numerical parameters used for the moment-method spray model used for this study are the same as those found in the experimental and numerical work Li [20] wherever possible. This is to allow a reasonable comparison of the performance of the moments-method spray model. In the DMF fuel spray simulation studies performed by Li [20] and Li *et al*. [8], the KIVA-3V code was used. The thermodynamics properties of the DMF fuel were added and the boundary conditions modified to correspond to the experiments from Li [20]. Several atomization and droplet breakup models were evaluated and the Cascade Atomization and Drop Breakup (CAB) and the Max Planck Institute (MPI) breakup models were found suitable for the simulation studies. The computational space was a constant volume cylindrical chamber with the numerical grid consisting of 40,000 computational cells.

For the moments-method spray model, the computational grid used is as presented in Figure (1). The fuel properties applied to the model are as presented in Table (1). The injector used, according to [20], is a 6-hole gasoline direct injection injector, but no other specification was given. From [19] it was inferred that this was a Bosch type injector and from the inlet Reynolds and Weber number values presented, nozzle diameter values of 0.132 mm and 0.182 mm, respectively, are possible. The earlier value was used in this study. For the moments-method spray model, the injection velocity of the liquid fuel is calculated using the Bernoulli argument:

$$U_{inj} = C_D \left[\frac{2\left(P_{inj} - P_g\right)}{\rho_l} \right]^{\frac{1}{2}} \tag{5}$$

where the coefficient of discharge (C_D) is taken as 0.7 as no experimental values were available.
The spray angle values for the three cases were estimated from the data in [20]. No inlet droplet diameter values were presented in [20]; these are needed in the moments-method spray model, however. Therefore, the procedure used in [9, 16] to estimate the inlet droplet diameter based on similar inlet conditions is used. Table (2) presents the parameters used for the simulation.

Parametric Tests
The parametric tests are based on the experimental data from [20], Case 1 from Table (2). These tests offer the evaluation of the capabilities of the moments-method spray model with respect to the effects of the ambient pressure values, and droplet sizes on the DMF fuel spray tip penetration predictions.

Table 2. Numerical, physical and injection parameters used to simulate the experiments of Li [20].

	Numerical Case 1	**Numerical Case 2**	**Numerical Case 3**
Injection pressure, (MPa)	5.0	5.0	5.0
Ambient pressure, (MPa)	0.1	0.3	0.6
Number of cells in axial x radial directions	109 x 73		
Injection velocity, (m/s)	Equation (5)		
Computational time step, (μs)	0.5		
Total computation time, (ms)	2.0		
Nozzle diameter, (mm)	0.132		
Spray angle	10°	16°	21°

Grid independency tests
The effect of changing the grid size on the fuel spray tip penetration has been extensively tested previously [9, 10]. With grid cell numbers increased with the ratios 1.0:2.5:4.0, the fuel spray tip penetration predictions were found to be insensitive to these grid sizes. Because of the need to capture spray tip values the larger grid size is used here (Figure (1)). The grid is non-uniform and about 70 % of the cells are in the region bordering the centreline to capture the dense spray regions of the fuel spray centreline. One feature of the moments-method spray model is the ability to specify the size of the injection cell with respect to the rest of the grid cells [16]. The maximum size of the injection cell (in the axial direction) was varied from 1.0 mm to 0.3 mm. Figure (2) presents the outcomes describing the effects of the injection cell grid density on the fuel spray tip penetration. The predictions indicate that the results are unaffected by when the grid is refined below 0.5mm. An injection cell size of 0.5 mm is used in this study.

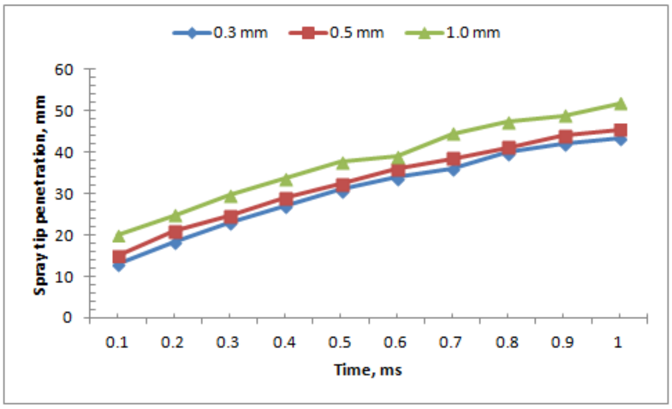

Figure 2. Variation of fuel spray tip penetration with the injection cell grid density at 0.1 MPa ambient pressure and 5.0 MPa injection pressure.

Variation of the Fuel Spray Tip Penetration with the Initial Droplet size values

Figure (3) presents the predictions of the fuel spray tip penetration with injection time for different inlet droplet size values. The results indicate that the fuel spray tip penetration is further throughout the injection time for when initially larger sized droplets are prescribed at the start of injection. Because of the effect of larger aerodynamic forces on smaller sized droplets, compared to the larger sized ones, they are slowed down at a faster rate than the larger sized droplets. Hence, the larger sized droplets travel further. The model captures this phenomenon.

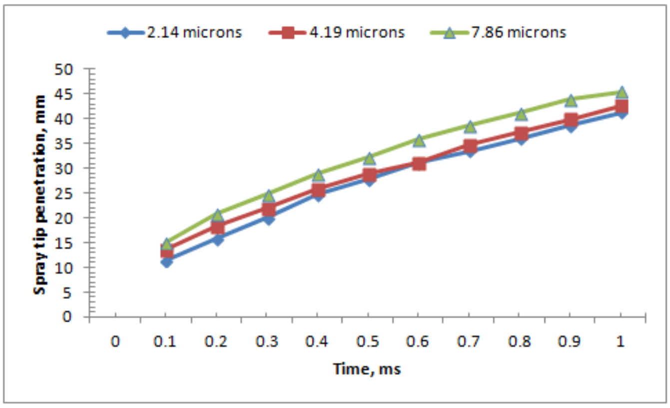

Figure 3. Variation of fuel spray tip penetration with the inlet droplet sauter mean radius at 0.1 MPa ambient pressure and 5.0 MPa injection pressure.

Comparison with Experimental data and Discrete-Droplet-Model results

The numerical results from the moments-method model are compared with the experimental and numerical data from the work of Li [20]. The experiments were conducted under room temperature (20ºC) conditions.

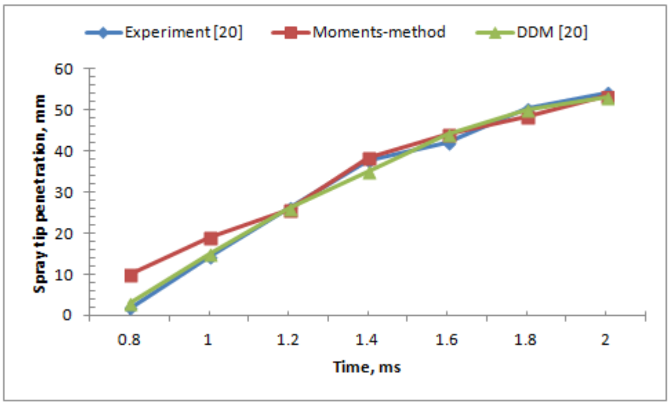

Figure 4. Comparison of predicted, experimental and DDM code spray tip penetration values at 0.1 MPa ambient pressure and 5.0 MPa injection pressure.

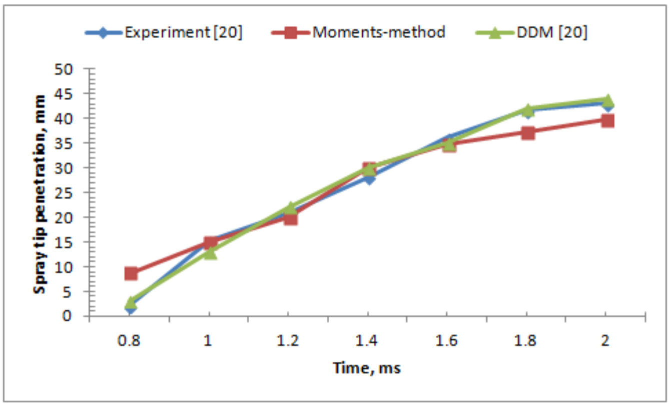

Figure 5. Comparison of predicted, experimental and DDM code spray tip penetration values at 0.3 MPa ambient pressure and 5.0 MPa injection pressure.

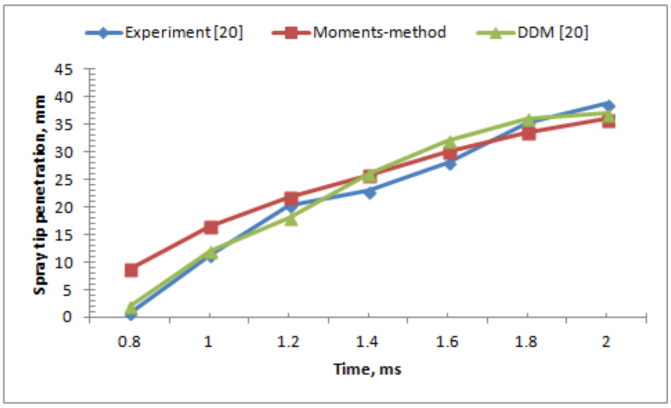

Figure 6. Comparison of predicted, experimental and DDM code spray tip penetration values at 0.6 MPa ambient pressure and 5.0 MPa injection pressure.

Figures (4 – 6) show the comparison of the predicted DMF fuel spray tip penetration with experimental data and predictions from a discrete-droplet-model (DDM) for ambient pressure values of 0.1, 0.3 and 0.6 MPa respectively. Results from the predicted values indicate that the DMF fuel spray tip increases as the fuel injection event progresses. As the duration of the fuel injection event increases, the fuel spray droplets travel further away from the injector nozzle until the initially high kinetic energy of the fuel liquid jet is dissipated due to frictional losses to the surrounding gas. The maximum distance that the spray tip can reach depends on the initial kinetic energy of the fuel spray as it emanates from the injector and the resistance to this from the surrounding gas. The predicted DMF fuel spray tip penetration captures this phenomenon; however, there are discrepancies in the quantitative predictions. The model predicts high fuel spray tip penetration initially whereas experimental data indicate shorter fuel spray tip penetration at the initial stages of injection. Some of the injection conditions were not available, including the initial droplet size distributions for the experiments and the DDM code [20], so the treatment for the initial droplet size distribution is as described in the 'Numerical Parameters' section. Therefore, the comparisons of the fuel spray tip penetration data from the end of the breakup period might be more meaningful in these instances. The definition of the spray penetration that has been used for the moments-method spray model presented here is the value of the furthest axial distance along the spray centreline in which there is any volume of liquid present or the point behind which 99% of the spray mass is located [16]; no definition was presented for the DDM model [8, 20].

The figures also show the evolution of the DMF fuel spray tip penetration with increases in ambient pressure. This is particularly clear from Figure (7). The predicted results correctly show that the DMF spray tip penetration decreases as the ambient pressure is increased. Given the same initial kinetic energy of the fuel spray as it emanates from the injector, higher carrier gas pressure values present greater frictional losses to the fuel spray and the maximum fuel spray tip penetration falls therefore. Quantitatively, the model reasonably predicts the DMF fuel spray tip penetration at the end of injection for each gas ambient pressure case. No direct computational cost comparison between the DDM and moments method was possible in this study, but a previous study indicated that a two-moments method scheme is nearly twice as fast as a DDM one [21].

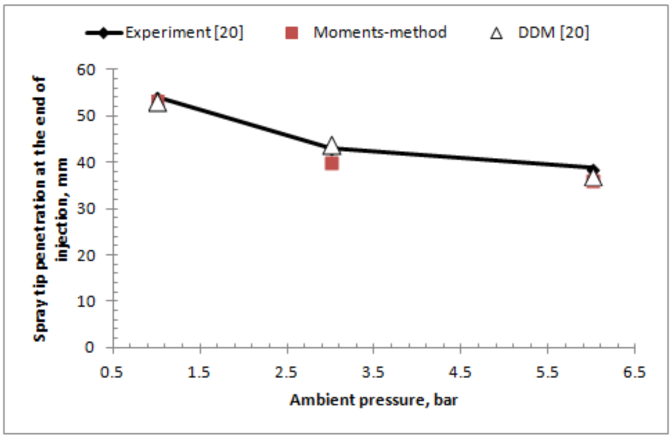

Figure 7. Comparison of predicted, experimental and DDM code spray tip penetration at the end of injection (2 ms) for the three ambient pressure cases. Injection pressure is 5.0 MPa for each case.

Conclusions

This study presented the application of a moments-based spray model to the prediction of the hydrodynamics of 2, 5-Dimethylfuran (DMF) fuel spray. The novelty of the moments-method spray model is that the complete hydrodynamics of sprays can be captured by calculating the moments of the droplet size distribution function. This is unlike the typical spray models (DDM) that usually must predict the chaotic motions of groups of identical droplets to present the hydrodynamics nature of sprays.

The results from the simulations were compared with experimental data and predictions from a DDM code. The results indicate that the DMF fuel spray tip penetration decreases with increasing ambient pressure values. This is as expected since higher ambient pressure values offer greater frictional resistance to travelling fuel spray droplets and the maximum fuel spray tip penetration decreases because of this. Quantitatively, the model does not capture the fuel spray tip penetration before the breakup period. This may be due to the treatment of some of the injection conditions which were unavailable from the experimental and DDM code. The use of similar injection conditions would help to assess the model at these periods of fuel injection. The model captures the fuel spray tip penetration data from after the breakup period.

The study of the hydrodynamic characteristics of biofuels such as 2, 5-Dimethylfuran can be greatly aided by using numerical simulations to complement experimental work, thus, offering extensive parametric studies at lower costs. The moments-method spray model is applicable to such studies.

Definitions/Abbreviations

$n(r)$	Number Size Distribution
Q	Droplet Moment
Q_0	Total Number
Q_1	Sum of Radii [m]
Q_2	Sum of Squares of Radii [m^2]
Q_3	Sum of Cubes of Radii, [m^3]
r	Radius [m]
S	*Source Term*
t	Time [s]
U	Velocity [m/s]
V	Volume [m^3]
x	Coordinate Direction [m]

Acronyms

DDM	Discrete Droplet Model
DMF	2, 5-dimethylfuran
DISI	Direct Injection Spark Ignition
GDI	Gasoline Direct Injection

Greek Symbols

μ	Dynamic viscosity [kg m^{-1}s^{-1}]
ρ	Density [kg m^{-3}]
σ	Surface tension [Nm^{-1}]

Subscripts

32	Sauter mean radius
g	Gas
i	Moment index
inj	Injection
j	Vector index
l	Liquid

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