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APPLICATION OF A LAMINAR FLAMELET COMBUSTION MODEL TO LPG AND DIESEL SPRAYS

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Abstract

The use of direct injection liquefied petroleum gas (LPG) in internal combustion engines poses possible fuel savings as well as reduced emissions of HC and CO. In direct injection, the development of the liquid fuel spray and its evaporation in the combustion chamber plays a key role in determining the quality of the subsequent combustion. In this study, the Discrete Droplet Model (DDM) is used together with the Kelvin-Helmholtz wave break up model and a modified evaporation model, to simulate LPG sprays. To account for combustion of fuel vapour and oxygen, a modified form of the laminar flamelet model has been implemented. Qualitative experimental data on LPG and diesel spray flames are used to support the results of the simulations.

Introduction

The need for more fuel efficient and environmentally friendly vehicles has been growing due to the increasingly stringent emission regulations as well as growing public awareness. The use of alternative fuel such as LPG could provide a number of advantages over conventional fuel. LPG consists of butane (C_4H_{10}) or propane (C_3H_8) or a mixture of both. It is a by-product of crude oil refining and thus the proportion of butane and propane depends largely on the country of origin [1].

LPG has a simple chemical composition. Therefore it enables complete combustion to be achieved more easily, resulting in lower emissions of HC and CO. Moreover, the fuel has a high octane rating, typically 112 RON for pure propane, which prevents the occurrence of ‘knocking’ at high engine compression ratio. With a high compression ratio, thermal efficiency can be improved thus resulting in fuel economy. LPG is not a new fuel in the automotive industry, as it has been utilised in dual fuel passenger cars as well as commercial vehicles, although the number is limited [2].

Most current LPG vehicles however use either carburetted fuel distribution or multi port (MPI) fuel injection systems. With direct injection, better fuel efficiency could be achieved due to the ability to control the amount and timing of fuel injection. However with direct injection, knowledge of the fuel spray characteristics becomes essential to ensure proper air and fuel vapour mixing. The successful implementation of gasoline direct injection (GDI) [3] relies on careful piston geometry design to produce the desired spray characteristics in order to obtain a stratified charge around the spark plug during lean combustion. The work described in [4] aimed to extend spray modelling methods to LPG fuel in order to predict its evaporating and non-evaporating sprays characteristics. Here this work is augmented by applying a recently extended model of combustion in order to assess its applicability to both LPG and diesel combustion simulations.

Mathematical Models

The finite volume method is used to discretize the gas phase transport equations. The Discrete Droplet Model (DDM) as described in [5] is used to model the fuel spray. The drop break-up is accounted for by the Kelvin-Helmholtz wave break-up model [6] while drop collisions are modelled using [7]. The EPISO algorithm, as extended in [1] to also calculate the spray equations, is used for the combined solution of the gas phase and spray equations.

During direct injection the major difference between LPG and conventional fuels, including gasoline and diesel, is that under certain possible engine conditions the LPG will flash evaporate. To account for this effect, the heat and mass transfer equations were extended, as described in [4].

This paper concentrates on the modified laminar flamelet model (LFM) of Ranasinghe and Cant[8] used to predict LPG and diesel spray combustion. One of the key assumptions in this model is that chemical reaction takes place only in the fuel vapour state. Therefore the liquid drops are allowed to continue to evaporate, using the evaporation model discussed in [4], while the reaction takes place in the surrounding fuel vapour and air mixture. In order to simplify the complex nature of combustion, the reaction is assumed to be a single step one given by:

$$1\,\text{kg Fuel} + s\,\text{kg Oxygen} \rightarrow (1+s)\,\text{kg Product} + Q(\text{heat}) \qquad (1)$$

where s is the stoichiometric ratio of the reaction and Q is the heat released from the chemical reaction.

This simplified chemical reaction equation identifies 4 separate mass fractions in the gas mixture, namely those for the fuel vapour Y_f, oxygen Y_o, inerts (assumed to be purely nitrogen) Y_{in} and the combustion product Y_p. Since these four species constitute the whole gas mixture, the sum of these mass fractions is unity. The mass fractions Y_o and Y_{in} can be expressed in terms of Y_f and the mixture fraction Z, by:

$$Y_O = A_{OX}(1 - z) + s(Y_f - Z) \tag{2}$$

$$Y_{in} = (1 - A_{ox})(1 - Z) \tag{3}$$

where $A_{ox} = 0.232$ is the mass fraction of oxygen in air.

Thus equations need only be solved for Y_f and Z. In the LFM a transport equation is not solved for Y_f. Instead one is solved for the density-weighted or Favre averaged progress variable $\tilde{c}$, which takes the value 0 in reactants and 1 in products. This transport equation is:

$$\frac{\partial(\rho\theta\tilde{c})}{\partial t} + \frac{\partial}{\partial x}(\rho\theta U\tilde{c}) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho\theta V\tilde{c}) = \frac{\partial}{\partial x}\left(\mu_{eff}\theta\frac{\partial\tilde{c}}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{eff}\theta\frac{\partial\tilde{c}}{\partial r}\right) + \overline{\omega} \tag{4}$$

where θ is the void fraction due to the presence of liquid in the gas phase computational volumes and the reaction rate $\overline{\omega}$ represents the consumption of fuel vapour during chemical reaction. A very similar equation is solved for the mixture fraction, except that there is no reaction rate term but there is a fuel vapour mass source from droplet evaporation. Values of Y_f are then obtained as outlined below.

In the conventional LFM a probability density function (pdf) is used to describe the combustion of a premixed, homogenous mixture of mixture fraction Z_{st}, where subscript *st* denotes stoichiometric conditions. During spray combustion, the mixture fraction is not homogenous throughout the combustion chamber, as the mixture fraction distribution is influenced by the gas and liquid motions and rate of evaporation of the spray drops. To include the mixing effects of the fuel, [8] extended the existing pdf to contain the mixture fraction. The expression for the joint pdf becomes:

$$P(c,T,Z;x,t) = \alpha(x,t)\delta(c)\delta(T - T_p)f_r(Z;x,t) + \beta(x,t)\delta(1-c)f_p(T)f_p(Z) \tag{5}$$

where T is the temperature.

The beta function is used to model the pdf of the mixture fraction as it is one of the most convenient and suitable forms of pdf. Hence the Favre averaged pdf of mixture fraction is given by:

$$\tilde{P}(Z;x) = \tilde{f}_p(Z) = C\tilde{Z}^{a-1}(1-\tilde{Z})^{b-1} \tag{6}$$

$C = 1/\beta(a,b)$ is the normalising parameter where the beta function is defined by:

$$\beta(a,b) = \int_0^1 z^{a-1}(1-z)^{b-1}dz = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} \tag{7}$$

and $\Gamma(a)$ defines the gamma function for which tabulated results can be obtained from Abramowitz and Stegun [9]. The variables a and b are defined as:

$$a = \tilde{Z}\left(\frac{(1-\tilde{Z})\tilde{Z}}{\tilde{Z}''^2} - 1\right) \text{ and } b = (1-\tilde{Z})\left(\frac{(1-\tilde{Z})\tilde{Z}}{\tilde{Z}''^2} - 1\right) \tag{8}$$

where $\tilde{Z}''^2$ is the mixture fraction variance.

The model defines the heat release parameter as:

$$\bar{\tau} = \frac{\bar{\rho}_r}{\bar{\rho}_p} - 1 \tag{9}$$

where $\bar{\rho}_r$ and $\bar{\rho}_p$ are the conditional reactant and product densities respectively. The mean density is given by:

$$\bar{\rho} = \int_0^1 \int_{T_{\min}}^{T_{\max}} \rho P(c,T;x,t)dTdc = \alpha\bar{\rho}_r + (1-\alpha)\bar{\rho}_p \tag{10}$$

The mean quantity of the progress variable $\bar{c}$ is given by:

$$\bar{c} = \int_0^1 \int_{T_{\min}}^{T_{\max}} cP\big(c,T;x,t\big)dTdc = \alpha \times 0 + (1-\alpha)\times 1 = (1-\alpha) = \beta \tag{11}$$

The Favre averaged progress variable $\tilde{c}$ is given by:

$$\tilde{c} = \frac{1}{\bar{\rho}} \int_0^1 \int_{T_{\min}}^{T_{\max}} c\rho P(c,T;x,t)dTdc = \frac{1}{\bar{\rho}}[(1-\alpha)x1x\bar{\rho}_p] = \frac{\bar{\rho}_p}{\bar{\rho}}\beta \tag{12}$$

Substituting (9) and (10) into the above equation leads to:

$$\beta = \frac{\tilde{c}(1+\bar{\tau})}{(\tilde{c}\bar{\tau}+1)}, \quad \frac{\bar{\rho}_r}{\bar{\rho}} = (1+\tilde{c}\bar{\tau}) \quad \text{and} \quad \frac{\bar{\rho}_p}{\bar{\rho}} = \frac{(1+\tilde{c}\bar{\tau})}{!+\bar{\tau}} \tag{13}$$

The mean reaction rate is calculated using the expression by Cant et al [10]:

$$\bar{\omega} = \bar{\rho}_r \tilde{u}_L^o \, \Sigma \tag{14}$$

where the mean surface to volume ratio Σ is calculated from the following expressions [11]:

$$\Sigma = \frac{\bar{c}(1-\bar{c})}{L_y} \qquad L_y = \frac{1}{C_o}\frac{\nu}{u_L^o}\left[\left(1 + C_f \frac{u'}{u_L^o}\right)\exp\left(-C_{I1}\left(\frac{u'}{u_L^o}\right)^{C_{I2}}\right)\right]^{-1} \tag{15}$$

The flame length scale L_y is seen to be a function of the gas-phase turbulence intensity u'. The model constants C_o, C_{I1}, C_{I2} and C_f are estimated to be 4.95x10^{-3}, 0.35, 0.5 and 4.45 respectively. These values are obtained by calibrating the model against experimental results of Cheng and Shepherd [12]. The unstretched laminar flame speed is expressed as a function of the equivalence ratio $\phi = \tilde{Z}/\tilde{Z}_{st}$ through an empirical correlation [13].

$$u_L^o(\phi) = A_1\phi^{A_2}\exp(-A_3(\phi - A_4)^2(T_r/T_{ref})^{A5}(p_r/p_{ref}\}^{A6} \tag{16}$$

The reference temperature and pressure in this correlation are 300 K and 1 atm respectively while the other model constants depend on the type of fuel used and are given in Abu-Orf [13] for a variety of fuels. The laminar flame speed is a function of equivalence ratio and is therefore a function of the mixture fraction. To obtain the Favre averaged value, the above function is integrated over the beta function pdf of the mixture fraction:

$$\begin{aligned}\tilde{u}_L^o &= \int_0^1 u_L^o(\tilde{Z})P(\tilde{Z};x)d\tilde{Z} = \beta(a,b)^{-1}\int_0^1 u_L^o(\tilde{Z})\tilde{Z}^{a-1}(1-\tilde{Z})^{b-1}d\tilde{Z} \\ &= \beta(a,b)^{-1}A_1(T/T_{ref})^{A5}(p/p_{ref})^{A6}\int_0^1 \phi^{A_2}\exp(-A_3(\phi - A_4)^2)\tilde{Z}^{a-1}(1-\tilde{Z})^{b-1}d\tilde{Z}\end{aligned} \tag{17}$$

A transport equation is needed for the mixture fraction variance $\tilde{Z}''^2$, which is required in determining the probability density function of the mixture fraction, equation (8):

$$\frac{\partial(\bar{\rho}\theta\tilde{Z}''^2)}{\partial t} + \frac{\partial}{\partial x}(\bar{\rho}\theta U\tilde{Z}''^2) + \frac{1}{r}\frac{\partial}{\partial r}(r\bar{\rho}\theta V\tilde{Z}''^2) = \frac{\partial}{\partial x}\left(\mu_{eff}\theta\frac{\partial\tilde{Z}''^{2^2}}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{eff}\theta\frac{\partial\tilde{Z}''^2}{\partial r}\right) + \theta(G - D) \tag{18}$$

This transport equation is similar in form to the turbulence kinetic energy transport equation where *G* is the production of the intensity of the mixture fraction due to turbulence while *D* is the dissipation of this parameter. Here *G* and D are defined as:

$$G = -2\left(\overline{\rho u''Z''}\frac{\partial\tilde{Z}}{\partial x} + \overline{\rho v''Z''}\frac{\partial\tilde{Z}}{\partial r}\right) = 2\mu_{eff}\left[\left(\frac{\partial\tilde{Z}}{\partial x}\right)^2 + \left(\frac{\partial\tilde{Z}}{\partial r}\right)^2\right] \qquad D = \bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Z}''^2 \tag{19}$$

where u”, v'', $\tilde{k}$ and $\tilde{\varepsilon}$ are the Favre-averaged values of velocity fluctuations, turbulent kinetic energy and its dissipation rate respectively.

Once $\tilde{c}$ and $\tilde{Z}$ are known, $\bar{Y}_f$ can be calculated from:

$$\bar{Y}_f = \frac{\bar{Y}_{f,r}(1 - \tilde{c}) + \bar{Y}_{f,p}\tilde{c}(1 + \bar{\tau})}{!+\tilde{c}\bar{\tau}}, \text{ where } \bar{Y}_{f,r} = \tilde{Z}, \quad \bar{Y}_{f,p} = \max(0.0, \frac{\tilde{Z} - \tilde{Z}_{st}}{1 - \tilde{Z}_{st}}) \tag{20}$$

Combustion Simulations

To date the modified LFM has only been applied to simulate the combustion of non-stoichiometric but pre-mixed mixtures of fuel and air. It has not been applied to spray combustion in which the fuel and air is only partially mixed and the mixture is evolving as the spray evaporates.

The spray combustion experiments simulated here were carried out in [14] by injecting the fuel spray into a constant volume bomb and impinging the fuel spray on a heated wall, perpendicular to the direction of the spray. After a period of ignition delay, the spray self ignites and the combustion reaction begins. The photographs of the experiments show that ignition does not always occur symmetrically, which is probably inevitable due to non-ideal experimental conditions. However, in order to simplify the simulation, ignition is assumed to occur symmetrically around a circular ring that is estimated, based on the experimental photographs, to be 0.01 m from the centre line. Fuel self-ignition is not simulated, instead ignition is prescribed by inserting an artificial heat source term in the computational cells forming the ignition ring. This gives rise to the chemical reaction when the fuel vapour mass fraction reaches the stoichiometric ratio. The details of the test cases investigated are shown in Table 1.

For Test Case 2, the experimental flame obtained is relatively symmetrical, as shown in Figure 1. The equivalent simulated results in Figure 2 indicate a fairly similar flame thickness as for the experiments. The photograph is taken through a round insert in the side of the bomb, allowing limited optical access. Thus not all the flame can be seen. This may account for some of the differences evident between the predictions and experiment, particularly at the edge of the flame on the cylinder wall. The simulated results also predict that no chemical reaction is taking place in the core of the spray, which is indicated by the lower temperatures in that region. The photograph is of the surface of the flame while the predicted results show a cross-section. The simulated results are plausible because the core of the spray is a region of high fuel vapour and low oxygen mixture that does not encourage chemical reaction.

Predicted results for Test Cases 1 and 3 show a similar level of agreement with experiment, although the experimental flame is less symmetric in Test Case 1 [15]. The predictions also capture the speeding up of the combustion process with injection into a higher-pressure mixture. The higher pressure results in more mass of oxygen being available for combustion. The peak temperatures also increase.

Results for Test Case 4, which is for diesel fuel, show a level of agreement between the predictions and experiment that is roughly similar to those for LPG, indicating that the modified LFM is applicable to both types of fuel [15]. The combustion rate for diesel is shown by the experiments to be substantially faster than that for LPG under similar conditions of pressure and temperature. This effect is captured in the simulations by changing the fuel properties, the heat released and the model constants in the laminar flame speed equation (16).

Conclusions

A new form of the laminar flamelet model of combustion has been implemented to solve for the combustion of oxygen with fuel vapour that has come from the evaporation of liquid sprays. This is the first known application of such a model to simulate spray combustion, and in particular to the study LPG spray combustion. The results indicate that both LPG and diesel spray combustion can be calculated with a good degree of success, although quantitative data are lacking in order to make firm conclusions at this stage in the development of the work. Apart from the fuel properties and heat released, only the laminar flame speed correlation needs to be adjusted to switch from one fuel to another.

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Test Case	1	2	3	4
Fuel Type	LPG			Diesel
Nozzle Diameter (mm)	0.22			
Nozzle Type	Single Hole			
Trapped Temperature (K)	500			
Trapped Pressure (MPa)	0.4	0.7	1.0	0.7
Injection Pressure (MPa)	10.0			
Initial Liquid Temperature (K)	280			
Wall Temperature (K)	789			
Distance of Wall from Injector (mm)	105			

Table 1. Spray Combustion Test Case Details

LPG Flame:
Initial Trapped Pressure = 0.7 MPa
Fuel Injection Pressure = 10 MPa

Figure 1. Flame photograph at 17.82 ms after ignition

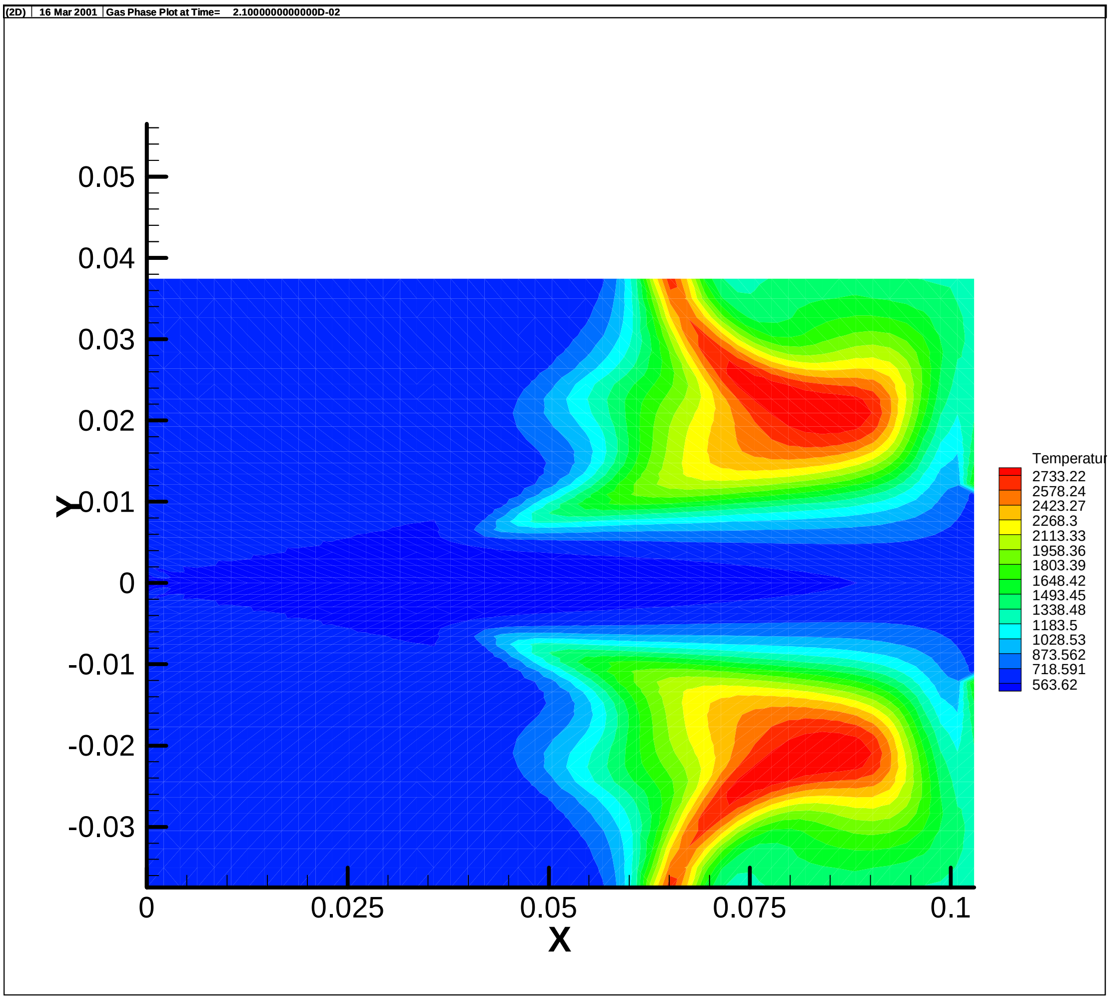

Figure 2. Simulated temperature contours 18 ms after ignition