B. TECH. PROJECT REPORT On A Vaporization Model for Discreet Multi-component Fuel Sprays

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A Vaporization Model for Discreet Multi-component Fuel Sprays

A PROJECT REPORT

Submitted in partial fulfillment of the requirements for the award of the degrees

of BACHELOR OF TECHNOLOGY in

MMECHANICAL ENGINEERING

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Guided by:

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CANDIDATE'S DECLARATION

We hereby declare that the project entitled **A Vaporization Model for Discreet Multi-component Fuel Sprays** submitted in partial fulfillment for the award of the degree of Bachelor of Technology in Mechanical Engineering completed under the supervision of **Dr. Devendra L. Deshmukh, Head of Department, Discipline of Mechanical Engineering,** IIT Indore is an authentic work.

Further, I/we declare that I/we have not submitted this work for the award of any other degree elsewhere.

Md Asim Azim

Monarch Joshi

Date:

CERTIFICATE by BTP Guide(s)

It is certified that the above statement made by the students is correct to the best of my/our knowledge.

Dr. Devendra L. Deshmukh

Head of Department

Discipline of Mechanical Engineering, IIT Indore

Date:

Date:

Preface

This report on A Vaporization Model for Discreet Multi-component Fuel Sprays is prepared under the guidance of Dr. Devendra L. Deshmukh. Through this report we have tried to design a mathematical model of evaporation of single as well as multi-component fuels and also, explored the effect of ambient pressure/density in evaporation of such fuels.

We have tried to the best of our abilities and knowledge to explain the content in a lucid manner.

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We are thankful to and fortunate enough t get constant encouragement, support and guidance from B. Tech project evaluation committee.

It is their help and support, due to which we became able to complete the design and technical report.

Abstract

The report throws light on vaporization of fuel droplets inside a combustion chamber of an internal combustion engine. Detailed study of aspects and assumptions of how to numerically determine the vaporization of fuels is explained in this report. Discreet multi-component modeling approach is used to formulate the vaporization model. This report also includes a brief study of fuels and their surrogate fuels to ease the computational load along with possessing some specific accuracy level. An approximate solution to the quasi-steady energy equation was used to derive an explicit expression for the heat flux from the surrounding gas to the droplet–gas interface, with inter-diffusion of fuel vapor and the surrounding gas taken into account. The density change of the drop as a function of temperature was also considered. In order to treat phase change under trans-critical conditions, a characteristic length was defined to determine the amount of vaporized fuel as a function of time. Finally, the study was implemented in a mat-lab code to attain results.

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[A.2] Properties

Temperature dependent and temperature independent properties of all the components.

Chapter 1

Introduction

1.1 Introduction

The vaporization of droplets and sprays has been an issue of much interest for decades because of its significance in engineering applications. Along with experimental studies, substantial effort has been made to predict the behavior of vaporizing droplets and sprays numerically.

In internal combustion engine applications, the ranges of pressures and temperatures where fuel vaporization takes place is broad. In particular, the range of pressures and temperatures in port fuel injection (PFI) engines, gasoline direct injection (GDI) engines and homogeneous charge compression ignition (HCCI) engines with early injections is relatively low, whereas that in conventional compression ignition (CI) engines may be high enough that the critical state of the fuel needs to be considered.

For simplicity, fuels have been represented as a single component fuel in most multi-dimensional models. However, single component fuel models are not able to predict the complex behavior of the vaporization of multi-component fuels such gasoline and diesel.

The preferential vaporization of light-end components in multi- component fuels affects greatly the fuel distribution near the spray and cannot be represented by single component fuel models.

1.2 Why are we modeling?

- Engines are basis of industry and modern human society
- Efficient engines are very necessary.
- Engines burn fuel. The level of combustion will determine engine's output.
- Level of combustion will depend on vaporization of fuels.
- Modeling of vaporization of fuels will not only increase output, but will also cause environment pollution due to improper and incomplete combustion of fuel.

1.3 Fuels

Fuels in consideration here are fossil fuels. Fossil fuels are hydrocarbons, primarily coal, fuel oil or natural gas, formed from the remains of dead plants and animals. The utilization of fossil fuels has enabled large-scale industrial development and largely supplanted water-driven mills, as well as the combustion of wood or peat for heat.

Fossil fuel is a general term for buried combustible geologic deposits of organic materials, formed from decayed plants and animals that have been converted to crude oil, coal, natural gas, or heavy oils by exposure to heat and pressure in the earth's crust over hundreds of millions of years.

The burning of fossil fuels by humans is the largest source of emissions of carbon dioxide, which is one of the greenhouse gases that allows radiative forcing and contributes to global warming.

A small portion of hydrocarbon-based fuels are bio-fuels derived from atmospheric carbon dioxide, and thus do not increase the net amount of carbon dioxide in the atmosphere.

Some fossil fuels:

[A] Gasoline: Gasoline or petrol is a derivative product of crude oil/petroleum. It is derived during fractional distillation process and has a translucent liquid form. It's not used in its crude form. Different additives are added like ethanol to use it as fuel for passenger vehicles. In the US and Latin countries, term gasoline is used, but in Europe and Asian countries it's called petrol.

[B] Diesel: Diesel fuel in general is any liquid fuel used in diesel engines, whose fuel ignition takes place, without any spark, as a result of compression of the inlet air mixture and then injection of fuel. Diesel engines have found broad use as a result of higher thermodynamic efficiency and thus fuel efficiency. This is particularly noted where diesel engines are run at part-load; as their air supply is not throttled as in a petrol engine, their efficiency still remains very high.

[C] Biodiesel: Fatty-acid methyl ester (FAME), more widely known as biodiesel, is obtained from vegetable oil or animal fats (bio-lipids) which have been transesterified with methanol. It can be produced from many types of oils, the most common being rapeseed oil (rapeseed methyl ester, RME) in Europe and soybean oil (soy methyl ester, SME) in the US. Methanol can also be replaced with ethanol for the transesterification process, which results in the production of ethyl esters. The transesterification processes use catalysts, such as sodium or potassium hydroxide, to convert vegetable oil and methanol into FAME and the undesirable

byproducts glycerin and water, which will need to be removed from the fuel along with methanol traces. FAME can be used pure (B100) in engines where the manufacturer approves such use, but it is more often used as a mix with diesel, BXX where XX is the biodiesel content in percent.

1.4 Fuel Surrogates

Fuel surrogates are mixtures of one or more simple fuels that are designed to emulate either the physical properties (vapor pressure) or combustion properties (laminar flame speed, heating value, etc.) of a more complex fuel. While surrogate mixtures can demonstrate more than one characteristic of the desired fuel, more often than not different components are required in order to emulate the wide variety of properties that are of interest to researchers. Jet fuel is an example of a fuel requiring a surrogate for experimental research and numerical modeling due to its complexity and high content variability from one batch to the next. Neat hydrocarbon jet fuel surrogate components include decane, dodecane, methylcyclohexane, and toluene. Gasoline surrogate components include n-heptane and iso-octane. Hexadecane is a diesel surrogate component. Biodiesel surrogate components include methyl butyrate and methyl decanoate.

1.5 Vaporization and Evaporation

Vaporization of an element or compound is a phase transition from the liquid phase to vapor. There are two types of vaporization: evaporation and boiling. Evaporation is a surface phenomenon, whereas boiling is a bulk phenomenon.

Evaporation is a type of vaporization of a liquid that occurs from the surface of a liquid into a gaseous phase that is not saturated with the evaporating substance. The other type of vaporization is boiling, which is characterized by bubbles of saturated vapor forming in the liquid phase.

Vaporization is a transitional phase of an element or compound from a solid phase or liquid phase to a gas phase while evaporation is a type of vaporization wherein the transition from a liquid phase to a gas phase takes place below the boiling temperature at a given pressure, and it occurs on the surface.

1.6 Modeling

Multi-component fuel models are classified into two types, i.e., discrete multi-component (DMC) models and continuous multi-component (CMC) models. The continuous multi-component model, which is based on the continuous thermodynamics method, represents the fuel composition as a continuous distribution function

with respect to an appropriate parameter such as molecular weight. This enables a reduction of computational load while maintaining the predictability of the complex behavior of the

vaporization of multi-component fuels. However, when this model is applied to combustion simulations, especially with detailed chemistry, describing the multi-component features of the fuel is inevitably limited, making it difficult to model the consumption

of individual components appropriately.

On the contrary, the DMC approach tracks the individual components of the fuel during the evaporation process and allows coupling with the reaction kinetics of the individual fuel components. Although the DMC approach can have a high computational overhead due to the additional transport equations that must be solved when it is used for fuels with a large number of components, it is becoming more affordable as computational capacity has improved substantially.

Chapter 2

Theoretical Formulation

2.1 Assumptions

- A spherically symmetric liquid droplet with a finite number of components vaporizing without chemical reactions in a gaseous environment is considered. Radiation and second order effects such as the Soret and Dufour effects are assumed to be negligible.
- With the fuel components treated as discrete species and assuming no absorption of the ambient gas into the liquid droplet, the system is a discrete system consisting of the liquid phase fuel species and a discrete mixture system of vapor phase fuel and ambient gas.
- The droplet evaporation rate predicted by conventional models is calculated by assuming that the surface temperature is equal to the droplet average temperature. This can lead to over-prediction or under-prediction of the evaporation mass flux, depending on the ambient temperature conditions.
- The liquid phase is approximated as being well mixed, since mass transfer rates of the components in the liquid droplets are large.
- Heat transfer rates are finite so the temperature in the droplet is not assumed to be uniform and a surface temperature model is introduced.
- The equilibrium at the interface between the liquid droplet and the surrounding gas is based on the assumption that the chemical potential for the liquid phase, and the vapor phase, are equal for each species. Assuming an ideal solution, the surface mass fraction of fuel vapor can be determined using Raoult's Law.
- Variation of liquid and vapor species mass fraction is assumed, so the mass fraction of fuel vapor at the surface is less than unity, and the concept of Spalding's mass transfer number is valid.
- Heating phenomenon is involved.

2.2 Numerical analysis and mathematical algorithm

The algorithm is explained step wise as below:

Step 1:

The rate of mass transport at the droplet surface is calculated using the well-known high mass transfer rate equation with Spalding's transfer number.

 $m = g_m \ln (B_m + 1)$

where,

m = rate of mass transfer per unit area and per unit time at the surface of the droplet

 $g_m = it \text{ is the mass transfer coefficient given by } \frac{Sh\rho\overline{D}}{2r}$ Sh = Sherwood Number $\rho = density \text{ of air including fuel vapours}$ $\overline{D} = average diffusion coefficient of fuel species$ r = radius of the droplet

And,

 $B_m = Spalding's transfer number given by below equation$

$$B_m = \frac{y_{Fs} - y_{Fsurr}}{1 - y_{Fs}}$$

where,

 $y_{Fs} = mass fraction of fuel at the surface$

 $y_{Fsurr} = mass \ fraction \ of \ fuel \ in \ the \ surrounding$

Diffusion coefficients are calculated using Fullers method,

$$\mathsf{D} = \frac{0.00143(\mathsf{T}_{\mathsf{avg}}^{1.75})}{P_{\sqrt{Ma_f}} (\left[A^{\frac{1}{3}} + B^{\frac{1}{3}}\right]^{\frac{2}{3}}}$$

where,

A = atomic diffusion volume of ambient gases

B = atomic diffusion volume of fuel vapours

And,

$$Ma_f = 2\left(\frac{1}{M_a} + \frac{1}{\theta_v}\right)^{-1}$$

 $M_a = Mean molecular weight of ambient gases$

 θ_v = Mean molecular weight of fuel vapours

Step 2:

Determination of surface temperature

 $L_{(Ts)} m = q_i + q_o$

$$q_i = h_{ieff}(T_d - T_s)$$
$$h_{ieff = \frac{K}{\delta}}$$

K = conductivity of liquid droplet

 $\delta = (\pi \chi \alpha t)^{0.5}$

 $\chi = 1.86 + 0.86 \text{tanh} [2.225 \log 10 (\text{Pe}/30)]$

 α = thermal diffusivity of liquid droplet

And,

$$q_{o} = h_{oeff}(T_{surr} - T_{sur})$$

$$h_{oeff} = \frac{kC_{p}m}{e^{Hoeff1 + Hoeff2 - 1}}$$
Hoeff1 = $\frac{2rC_{p}m}{KN_{u}}$
Hoefff2 = $\frac{C_{a}(y_{surr} - y_{sur})Sh}{KN_{u}}$
Where,
$$C_{a} = \rho(\overline{C_{pf}D_{f}} - C_{pa}\overline{D_{f}})$$

$$\rho = density of air including fuel vapor
$$C_{pf} = C_{p} offuel species$$

$$D_{f} = Diffusion coefficient offuel$$

$$C_{pa} = C_{p} of ambient air$$$$

Finally,

$$L_{(Ts)} m = h_{ieff}(T_d - T_s) + \frac{kC_pm}{e^{\frac{2rC_pm}{KN_u} + \frac{C_a(y_{surr} - y_{sur})Sh}{KN_u} - 1}}(T_{surr} - T_{sur})$$

In calculation of surface temperature, iteration method is used to arrive at the correct T_s . Initially, a particular value of T_s is assumed, and the values needed for the above equation is drawn out at this temperature. All the values are now fed to the equation to calculate T_s .

vapours

Finally, same formula is used again and again (iterated) until we get the correct T_s .

Step 3:

After the first time step, the physical aspects of the droplet must have changed. To calculate the new required properties following equations were used.

To find the new radius after each iteration:

$$\rho \frac{4}{3}\pi R_2^{3} = \rho \frac{4}{3}\pi R_1^{3} - m 4\pi R_1^{2} \Delta t$$

 Δt is taken as 1 milli second for the iterations in case of all the components.

To find new droplet temperature after each iteration:

$$C_{\nu}\rho \frac{4}{3}\pi R_{2}^{3}T_{d2} = C_{\nu}\rho \frac{4}{3}\pi R_{1}^{3}T_{d1} + 4\pi R_{1}^{2}(q_{i} - mC_{\nu}T_{s})\Delta t$$

To get all these values we need to know the concentration of the species of the droplet after each time step, which can be calculated as given below:

Using Raoult's Law;

$$P_{1\nu} = P_{sat1}x_1$$

where,

 P_{1v} = Partial pressure of coponent 1 in surrounding P_{sat} = Saturation pressure of component 1

 x_1 = mole fraction of component 1 in liquid droplet

Now, as partial pressure of each component is known, we can find out their mole fraction in the surrounding.

 y_1 = mole fraction of component 1 in surrounding = $\frac{P_{sat1}x_1}{\Sigma P_{sat1}x_1 + P_{amb}}$

$P_{amb} = Partial \ pressure \ of \ ambient \ gas$

Also, the total mass evaporated is known to us, so it can be multiplied with mass fraction of each fuel component in the surrounding to get the mass evaporated of each component. Then, mass evaporated can be subtracted from initial mass to get mass left and mole fraction can also be calculated.

Step 4:

Finally all these formulae and equations are repeated as required to formulate the evaporation of the droplet.

Chapter 3

Results and Discussions

[A] Results for single component evaporation model of tetra-decane:

(i) Variation of droplet and surface temperature:





[B] Mixture of dodecane and tetradecane

(i) Variation of droplet and surface temperature:





(iii) Droplet radius variation:



[C] Mixture of ethanol and methyl oleate:

(i) Effect of varying initial mole fraction of components and their change in the droplet with respect to time.





(ii) Effect of varying concentration of mixture on droplet temperature:











(i) Effect on mole fraction:









Chapter 4

Conclusion and Future Aspects

4.1 Conclusions

- Vaporization processes of multi-component automotive fuels were successfully simulated by the present DMC evaporation model for various evaporation conditions.
- Multi-component single droplet evaporation differs significantly from that of a single component fuel in terms of time histories of their respective vaporization constants and droplet life times.
- The variation of ambient temperature is also very influential. The rate of decrease of drop life time with respect to increases in the ambient temperature decreases with increasing ambient temperature.
- The initial drop temperature mainly affects the early stages of evaporation of single multi-component droplets. The evaporation constants during the later stages of the drop life time are independent of the initial drop temperature.
- The initial drop temperature mainly affects the early stages of evaporation of single multi-component droplets. The evaporation constants during the later stages of the drop life time are independent of the initial drop temperature.
- Preferential evaporation of the light-end components of multi component fuels increases the amount of light-end components upstream of the spray plume. On the contrary, the heavy-end components are found predominantly in the region near the tip of the spray.
- Pressure increase does not have a significant effect on the droplet lifetime.
- In the case of ethanol and methyl oleate, while changing mole fraction of ethanol, it was clearly seen that the droplet radius change was significant in the initial stage as it is highly volatile and it got evoparated completely and then since pressure was high rate of evaporation of methyl oleate was negligible.

4.2 Future Aspects:

- D² Law can be extended to bi-component evaporation model.
- Bi-component DMC model can be extended to multi-component models, subsequently using real fuels instead of surrogate fuels.
- Highly accurate models will not only help in understanding vaporization of fuels more efficiently, but will also help in building better engines with high efficiency.
- Ultimately, engines with better output and low emissions will be made.

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- (4) http://app.knovel.com/knovel2/HTML_Link.jsp?Filename=1187/dsa/svp/dsa_a_svp_1102_page_1.ht m&htmlBookID=1187/cid
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Appendix

[A.1] Matlab Code

% component 1 = n-dodecan % component 2 = n-tetradecane

- % Surrounding gases contains only nitrogen therefore mean molecular weight of ambient gas is 28u.
- % Surrounding pressure is 1 bar = Partial prssur of nitrogen and tempreture is 500k.
- % Initial droplet tempreture is 360 K.

% initial diameter of droplet is 100 micro meter.

clc

Tsurr = 400;

Td0 = 320;

Tcd = 657;% critical tempreture

Tct = 691;

Tce = 513.92;

Tcoa = 781;

Tcmo = 764;

 $Ts1 = (1.1)^* Td0$; % It is the initial assumed surface tempreture

 $r_0 = 50*(10^-6);$

 $dt = 10^{(-3)};$

Tfinal = $180*(10^{-3})$;

x1 = 0;

x2 = 0;

x3 = 0.5;

x4 = 0;

x5 = 0.5;

% calculation of liquid density

 $Rho1 = (0.33267/(0.24664^{(1+(1-Td0/658)^{0.28571})))*170.34; \% (kg/m3)$

 $Rho2 = (0.27248/(0.24007^{(1+(1-Td0/693)^{0.28571})))*198.394;$

 $Rho3 = (1.6288/(0.27469^{(1+(1-Td0/514)^{0.23178})))*46.06844;$

 $Rho4 = (0.26668/(0.26667^{(1+(1-Td0/781)^{0.30687}))) * 282.46136;$

 $Rho5 = (0.24755/(0.2624^{(1+(1-Td0/764)^{0.33247})))*296.48794;$

Rho = x1*Rho1 + x2*Rho2 + x3*Rho3 + x4*Rho4 + x5*Rho5;

% Calculation of liquid mass

Mass_droplet_initial =($Rho^{4}^{3.14}(r_0^{3}))/3$;

```
Mass_dodecane_initial = ((Mass_droplet_initial)*170.34*x1)/(170.34*x1+198.394*x2+46.06844*x3+282.46136*x4+296.48794*x5);
```

Mass_tetradecane_initial = ((Mass_droplet_initial)*198.394*x2)/(170.34*x1+198.394*x2+46.06844*x3+282.46136*x4+296.48794*x5);

Mass_ethanol_initial = ((Mass_droplet_initial)*46.06844*x3)/(170.34*x1+198.394*x2+46.06844*x3+282.46136*x4+296.48794*x 5);

Mass_oa_initial = ((Mass_droplet_initial)*282.46136*x4)/(170.34*x1+198.394*x2+46.06844*x3+282.46136*x4+296.48794*x5);

Mass_mo_initial =

 $((Mass_droplet_initial)*296.48794*x5)/(170.34*x1+198.394*x2+46.06844*x3+282.46136*x4+296.48794*x5);$

for i=1:180

$$Ts1 = 1.01 * Td(i-1);$$

else

Ts1 = 1.01 * Td0;

end

disp(Ts1)

 $r_0 = 50*(10^{(-6)});$

if i>1

 $Psat2 = \exp(140.47 - 13231/Td(i-1) - 16.859*log(Td(i-1)) + 0.0000065877*(Td(i-1)^{2})); \% \text{ psat is in pascal}$

 $Psat1 = \exp(137.47 - 11976/Td(i-1) - 16.698 \log(Td(i-1)) + 0.0000080906 (Td(i-1)^{2}));$

 $Psat3 = \exp(73.304 - 7122.3/Td(i-1) - 7.1424*\log(Td(i-1)) + 0.0000028853*(Td(i-1)^{2}));$

 $Psat4 = \exp(162.45 - 19053/Td(i-1) - 18.997*\log(Td(i-1)) + 0.0000042699*(Td(i-1)^{2}));$

 $Psat5 = \exp(187.49 - 19153/Td(i-1) - 22.989*\log(Td(i-1)) + 0.0000072769*(Td(i-1)^{2}));$

else

 $Psat2 = exp(140.47 - 13231/Td0 - 16.859*log(Td0) + 0.0000065877 * ((Td0)^2)); \%$ psat is in pascal

 $Psat1 = exp(137.47 - 11976/Td0 - 16.698*log(Td0) + 0.0000080906*((Td0)^{2}));$

Psat3 = exp $(73.304 - 7122.3/Td0 - 7.1424*log(Td0) + 0.0000028853*((Td0)^2));$

$$Psat4 = \exp(162.45 - 19053/Td0 - 18.997*\log(Td0) + 0.0000042699*((Td0)^2));$$

Psat5 = $\exp(187.49 - 19153/Td0 - 22.989 \cdot \log(Td0) + 0.0000072769 \cdot ((Td0)^2));$

end

if i>1 ;

 $P1v = x1(i-1)* Psat1*(10^{(-5)}); \quad \%(\text{ value is in bar})$ $P2v = x2(i-1)* Psat2*(10^{(-5)});$ $P3v = x3(i-1)* Psat3*(10^{(-5)});$ $P4v = x4(i-1)* Psat4*(10^{(-5)});$ $P5v = x5(i-1)* Psat5*(10^{(-5)});$

$$P6v = 1;$$

else

 $P1v = x1^* Psat1^*(10^{(-5)});$ %(value is in bar)

 $P2v = x2* Psat2*(10^{-5});$

P3v = x3* Psat3*(10^(-5));

 $P4v = x4* Psat4*(10^{-5});$

 $P5v = x5* Psat5*(10^{(-5)});$

P6v = 1; % partial pressure of nitrogen

end

Ptotal = P1v + P2v + P3v + P4v + P5v + P6v; % (in bar)

y1 = P1v / (Ptotal);

y2 = P2v / (Ptotal);

y3 = P3v/(Ptotal);

y4 = P4v/(Ptotal);

y5 = P5v/(Ptotal);

y6 = 1/(Ptotal);

% Calculation of density of air

% considering only nitrogen

R = 0.08314; % value is in l-bar/k-mole

M = 28; % doubt

rho = (P6v*M)/(R*Tsurr); % M is the average molecular mass of fuel vapour mixture. % (doubt)

% calculation of liquid density

if i>1

 $Rho1 = (0.33267/(0.24664^{(1+(1-Td(i-1)/658)^{0.28571})))*170.34; \% (kg/m3)$

 $Rho2 = (0.27248/(0.24007^{(1+(1-Td(i-1)/693)^{.28571})))*198.394;$

 $Rho3 = (1.6288/(0.27469^{(1+(1-Td0/514)^{.23178})))*46.06844;$

 $Rho4 = (0.26668/(0.26667^{(1+(1-Td0/781)^{.30687}))) * 282.46136;$

 $Rho5 = (0.24755/(0.2624^{(1+(1-Td0/764)^{.33247})))*296.48794;$

Rho = x1(i-1)*Rho1 + x2(i-1)*Rho2 + x3(i-1)*Rho3 + x4(i-1)*Rho4 + x5(i-1)*Rho5;

else

 $Rho1 = (0.33267/(0.24664^{(1+(1-Td0/658)^{0.28571})))*170.34; \% (kg/m3)$

 $Rho2 = (0.27248/(0.24007^{(1+(1-Td0/693)^{.28571})))*198.394;$

 $Rho3 = (1.6288/(0.27469^{(1+(1-Td0/514)^{.23178})))*46.06844;$

 $Rho4 = (0.26668/(0.26667^{(1+(1-Td0/781)^{.30687}))) * 282.46136;$

 $Rho5 = (0.24755/(0.2624^{(1+(1-Td0/764)^{.33247}))) * 282.46136;$

Rho = x1*Rho1 + x2*Rho2 + x3*Rho3 + x4*Rho4 + x5*Rho5;

end

% Conductivity of liquid droplet

if i>1

```
k1 = 0.20293 - (0.00021798*Td(i-1)); % (w/mk)
```

 $k^2 = 0.2047 - (0.0002326*Td(i-1));$

k3 = 0.2468 - (0.000264*Td(i-1));

k4 = 0.20833 - (0.00019277*Td(i-1));

k5 = 0.18723 - (0.000142*Td(i-1));

K = (x1(i-1)*k1) + (x2(i-1)*k2) + (x3(i-1)*k3) + (x4(i-1)*k4) + (x5(i-1)*k5);

else

k1 = 0.20293 - (0.00021798*Td0); % (w/mk)

 $k^2 = 0.2047 - (0.0002326*Td0);$

k3 = 0.2468 - (0.000264 * Td0);

k4 = 0.20833 - (0.00019277*Td0);

k5 = 0.18723 - (0.000142*Td0);

 $\mathbf{K} = (\mathbf{x1}^*\mathbf{k1}) + (\mathbf{x2}^*\mathbf{k2}) + (\mathbf{x3}^*\mathbf{k3}) + (\mathbf{x4}^*\mathbf{k4}) + (\mathbf{x5}^*\mathbf{k5});$

end

```
% Heat capacity of liquid droplet

if i>1

Cpliq1 = (508210 - (1368.7*Td(i-1)) + (3.10158)*(Td(i-1)^{(2)}))/170.34; % (J/kg-K)

Cpliq2 = (353140 - (29.13*Td(i-1)) + (0.86116)*(Td(i-1)^{(2)}))/198.394;

Cpliq3 = (102640 - (139.63*Td(i-1)) - (0.030341)*(Td(i-1)^{(2)}))/46.06844;

Cpliq4 = (459000 - (866*Td(i-1)) + (3.74)*(Td(i-1)^{(2)}))/282.46136;

Cpliq5 = (324000 + (928*Td(i-1)))/296.48794;

else

Cpliq1 = (508210 - (1368.7*Td0) + (3.10158)*(Td0^{(2)}))/170.34; % (J/kg-K)

Cpliq2 = (353140 - (29.13*Td0) + (0.86116)*(Td0^{(2)}))/198.394;

Cpliq3 = (102640 - (139.63*Td0) - (0.030341)*(Td0^{(2)}))/46.06844;

Cpliq4 = (459000 - (866*Td0) + (3.74)*(Td0^{(2)}))/282.46136;
```

end

if i>1

```
Cpliq = x1(i-1)*Cpliq1 + x2(i-1)*Cpliq2 + x3(i-1)*Cpliq3 + x4(i-1)*Cpliq4 + x5(i-1)*Cpliq5;
```

D1 = k1/(Rho1*Cpliq1); % (m2/sec) D is diffusivity

D2 = k2/(Rho2*Cpliq2);

D3 = k3/(Rho3*Cpliq3);

D4 = k4/(Rho4*Cpliq4);

D5 = k5/(Rho5*Cpliq5);

D = x1(i-1)*D1 + x2(i-1)*D2 + x3(i-1)*D3 + x4(i-1)*D4 + x5(i-1)*D5;

else

Cpliq = x1*Cpliq1 + x2*Cpliq2 + x3*Cpliq3 + x4*Cpliq4 + x5*Cpliq5;

D1 = k1/(Rho1*Cpliq1); % (m2/sec) D is diffusivity

D2 = k2/(Rho2*Cpliq2);

D3 = k3/(Rho3*Cpliq3);

D4 = k4/(Rho4*Cpliq4);

D5 = k5/(Rho5*Cpliq5);

D = x1*D1 + x2*D2 + x3*D3 + x4*D4 + x5*D5;

end

k = 2; % k is the corelation factor

% Vapour phase Heat capacity of dodecane and tetradecane assuming to be ideal

%(J/kg-k)

Cp1 = (212950 + 663300*((1715.5/Tsurr)/sinh(1715.5/Tsurr))^2 + 451610*((777.5/Tsurr)/cosh(777.5/Tsurr))^2)/170.34 ;

Cp2 = (230820 + 786780*((1682.3/Tsurr)/sinh(1682.3/Tsurr))^2 + 544860*((743.1/Tsurr)/cosh(743.1/Tsurr))^2)/198.394 ;

$$\label{eq:cp3} \begin{split} Cp3 = & (49200 + 145770*((1662.8/Tsurr)/sinh(1662.8/Tsurr))^2 + \\ & 93900*((744.7/Tsurr)/cosh(744.7/Tsurr))^2)/46.06844 \;; \end{split}$$

$$\label{eq:cp5} \begin{split} Cp5 = & (329970 + 971600*((1645.6/Tsurr)/sinh(1645.6/Tsurr))^2 + \\ & 674480*((748/Tsurr)/cosh(748/Tsurr))^2)/296.48794 \;; \end{split}$$

 $Cp4 = (320000 + 936200^{*}((1743.1/Tsurr)/sinh(1743.1/Tsurr))^{2} + 675400^{*}((782.5/Tsurr)/cosh(782.5/Tsurr))^{2})/282.46136;$

Cpn = 1056;

Cpavg = (y1*Cp1) + (y2*Cp2) + (y3*Cp3) + (y4*Cp4) + (y5*Cp5) + (y6*Cpn);

for j=1:100

% Calculation of density of air (including fuel vapours)

Mavg = y1*170.34 + y2*198.394 + y3*46.06844 + y4*282.46136 + y5*296.48794 + y6*28;

rho_avg = (Ptotal * Mavg)/(R*Tsurr);

% in kg/m3

Ad = 109620000;

Bd = 1.5544;

Cd = -1.5358;

Dd = -1.5358;

At = 120070000;

Bt = 1.445;

Ct = -1.3846;

Dt = 0.42836;

Trd = Ts1/Tcd;

Trt = Ts1/Tct;

Tre = Ts1/Tce;

Troa = Ts1/Tcoa;

Trmo = Ts1/Tcmo;

 $L_1 = (Ad* (1-Trd)*(Bd + Cd*Trd + Dd*(Trd^2)))/170.34; % L_1 is the latent heat of vapourisation. J/kg$

 $L_2 = (At^* (1-Trt)^* (Bt + Ct^*Trt + Dt^*(Trt^2)))/198.394;$

 $L_3 = (65831000* (1-Tre)*(1.1905 - 1.7666*Tre + 1.0012*(Tre^2)))/46.06844;$

 $L_4 = (193110000*(1-Troa)*(1.8467 - 2.2939*Troa + .94672*(Troa^2)))/282.46136;$

 $L_5 = (213770000*(1-Trmo)*(2.3882 - 2.873*Trmo + 1.0193*(Trmo^2)))/296.48794;$

% Tr represents reduced tempreture

if i>1

 $L_T = x1(i-1)*L_1 + x2(i-1)*L_2 + x3(i-1)*L_3 + x4(i-1)*L_4 + x5(i-1)*L_5$;% x1 and x2 are mole fractions of fuel components in liquid and L is the latent heat of vapourisation.

else

 $L_T = x_1*L_1 + x_2*L_2 + x_3*L_3 + x_4*L_4 + x_5*L_5;$

end

% Calculation of evoparated mass at each step

Sh = 7; % (to be changed)(it is dimensionless)

Nu = 2.2; % (to be changed)

% Calculation of diffusion coefficient.

Tavg = (2*Tsurr + Ts1)/3;

q = 0.00143*(Tavg^1.75);

Ma = 28;

hv1 = 170.34;

hv2 = 198.394; % y1 and y2 are mole fractions of dodecane and tetradecane respectively.

hv3 = 46.06844;

hv4 = 282.46136;

hv5 = 296.48794 ;

 $Maf1 = 2*(((1/Ma)+(1/hv1))^{-1});$ % Ma is the mean molecular weight of the ambient gases, hv is the mean molecular weight of the fuel vapour

 $Maf2 = 2*(((1/Ma)+(1/hv2))^{-1});$

 $Maf3 = 2*(((1/Ma)+(1/hv3))^{-1});$

 $Maf4 = 2*(((1/Ma)+(1/hv4))^{-1});$

Maf5 = $2*(((1/Ma)+(1/hv5))^{-1});$

A = 18.5; % (nitrogen) (cm3/mole)

B1 = 12*15.9 + 26*2.31; % (dodecane)

B2 = 14*15.9 + 30*2.31; % (tetradecane)

B3 = 2*15.9 + 5*2.31 + 6.11;

B4 = 18*15.9 + 34*2.31 + 2*6.11;

B5 = 19*15.9 + 36*2.31 + 2*6.11;

w1 = $(Maf1^{0.50}) * (((A)^{1/3}) + ((B1)^{1/3}))^2);$ % P is the pressure and A and B are sum of the atomic diffusion volumes comprising the ambient gases and

% the fuel vapour respectively.

 $w2 = (Maf2^{0.5}) * ((((A)^{1/3}) + ((B2)^{1/3}))^{2});$ $w3 = (Maf3^{0.5}) * ((((A)^{1/3}) + ((B3)^{1/3}))^{2});$ $w4 = (Maf4^{0.5}) * ((((A)^{1/3}) + ((B4)^{1/3}))^{2});$ $w5 = (Maf5^{0.5}) * ((((A)^{1/3}) + ((B5)^{1/3}))^{2});$ $DVT1 = (q/w1)^{*}10^{(-4)}; \% (m2/sec)$

 $DVT2 = (q/w2)*10^{(-4)};$

 $DVT3 = (q/w3)*10^{(-4)};$

DVT4 = $(q/w4)*10^{(-4)};$

DVT5 = $(q/w5)*10^{(-4)}$;

 $DVT_avg = (DVT3 + DVT5)/2;$

if i > 1

 $G = (Sh* rho_avg*DVT_avg)/(2*r(i-1)); % DVT is average diffusion coefficient and r is the droplet radius.$

 $G = (Sh* rho_avg*DVT_avg)/(2*r_0);$

end

$$\begin{split} H &= (y1*170.34 + y2*198.394 + y3*46.06844 + y4*282.46136 + y5*296.48794) / (y1*170.34 + y2*198.394 + y3*46.06844 + y4*282.46136 + y5*296.48794 + y6*28) ; \end{split}$$

Bx = (H)/(1-H); % H is mole fraction at surface of fuel vapour

m = G*log(1+Bx); %(kg/m2-sec)

% Calculation of hieff.

Pe = 200; % dimensionles

X = 1.86 + 0.86*tanh(2.225*log10(Pe/30)); % Pe is peklet Number

delta = $(3.14*X*D*.001)^{(0.5)}$;

hieff = K/delta ; % W/m2-K

hoeff1 = k*Cpavg*m ;

if i>1

```
hoeff2 = (2*r(i-1)*Cpavg*m)/(Nu*K);
```

else

hoeff2 = $(2*r_0*Cpavg*m)/(Nu*K)$;

end

```
\label{eq:hoeff3} \begin{split} & \mbox{hoeff3} = (CA^*(y2^*198.394 + y1^*170.34 + y3^*46.06844 + y4^*282.46136 + y5^*296.48794 \\ )^*Sh)/(K^*Nu^*(y2^*198.394 + y1^*170.34 + y3^*46.06844 + y4^*282.46136 + 296.48794^*y5 + 28^*y6)) \ ; \end{split}
```

```
hlow = exp(hoeff2+hoeff3)-1;
```

hoeff = (hoeff1/hlow) ; % W/m2-sec

if i<2

```
Ts = (hoeff*Tsurr + hieff*Td0 - m*L_T)/(hieff + hoeff);
```

else

```
Ts = (hoeff*Tsurr + hieff*Td(i-1) - m*L_T)/(hieff + hoeff);
```

end

display (Ts);

Er = abs(Ts1 - Ts); % Er is the error

if (Er>0.1)

Ts1 = Ts;

disp(Ts1)

else

break;

end

end

if i>1

```
Mass\_evoparated(i) = m*4*3.14*(r(i-1)^{2})*dt + Mass\_evoparated(i-1);
```

else

Mass_evoparated(i) = $m^{4}(r_{0})^{3}$;

end

Tsf(i)=Ts;

% Calculation of new radius.

if i>1

end

%Calculation of new Td0, Td02

if i>1

 $qi = -hieff^*(Td(i-1)-Ts);$

else

$$qi = -1*hieff*(Td0-Ts);$$

end

if i>1

```
Td(i) = ((r(i-1)/r(i))^3)^Td(i-1) + (3^*(r(i-1)^2)^*dt^*(qi-(m^*Cpliq^*Ts)))/(Rho^*Cpliq^*(r(i)^3));
```

display (i);

else

 $Td(i) = ((r_0/r(i))^3)^T Td0 + (3^*((r_0)^2)^* dt^*(qi-(m^*Cpliq^*Ts)))/(Rho^*Cpliq^*(r(i)^3));$

end

% Calculation of new x1 and x2

if i>1

```
Mass\_evoparated\_dodecane = (Mass\_evoparated(i)*x1(i-1)*Psat1*170.34)/(x1(i-1)*Psat1*170.34 + x2(i-1)*Psat2*198.394 + x3(i-1)*Psat3*46.06844 + x4(i-1)*Psat4*282.46136 + x5(i-1)*Psat5*296.48794);
```

 $Mass_evoparated_tetradecane = (Mass_evoparated(i)*x2(i-1)*Psat2*198.394)/(x1(i-1)*Psat1*170.34 + x2(i-1)*Psat2*198.394 + x3(i-1)*Psat3*46.06844 + x4(i-1)*Psat4*282.46136 + x5(i-1)*Psat5*296.48794);$

 $Mass_evoparated_ethanol = (Mass_evoparated(i)*x3(i-1)*Psat3*46.06844)/(x1(i-1)*Psat1*170.34 + x2(i-1)*Psat2*198.394 + x3(i-1)*Psat3*46.06844 + x4(i-1)*Psat4*282.46136 + x5(i-1)*Psat5*296.48794);$

 $Mass_evoparated_oa = (Mass_evoparated(i)*x4(i-1)*Psat4*282.46136)/(x1(i-1)*Psat1*170.34 + x2(i-1)*Psat2*198.394 + x3(i-1)*Psat3*46.06844 + x4(i-1)*Psat4*282.46136 + x5(i-1)*Psat5*296.48794);$

 $Mass_evoparated_mo = (Mass_evoparated(i)*x5(i-1)*Psat5*296.48794)/(x1(i-1)*Psat1*170.34 + x2(i-1)*Psat2*198.394 + x3(i-1)*Psat3*46.06844 + x4(i-1)*Psat4*282.46136 + x5(i-1)*Psat5*296.48794);$

 $Mass_evoparated_dodecane = (Mass_evoparated(i)*x1*Psat1*170.34)/(x1*Psat1*170.34 + x2*Psat2*198.394 + x3*Psat3*46.06844 + x4*Psat4*282.46136 + x5*Psat5*296.48794);$

 $Mass_evoparated_tetradecane = (Mass_evoparated(i)*x2*Psat2*198.394)/(x1*Psat1*170.34 + x2*Psat2*198.394 + x3*Psat3*46.06844 + x4*Psat4*282.46136 + x5*Psat5*296.48794);$

 $Mass_evoparated_ethanol = (Mass_evoparated (i)*x3*Psat3*46.06844)/(x1*Psat1*170.34 + x2*Psat2*198.394 + x3*Psat3*46.06844 + x4*Psat4*282.46136 + x5*Psat5*296.48794);$

 $Mass_evoparated_oa = (Mass_evoparated(i)*x4*Psat4*282.46136)/(x1*Psat1*170.34 + x2*Psat2*198.394 + x3*Psat3*46.06844 + x4*Psat4*282.46136 + x5*Psat5*296.48794);$

Mass_evoparated_mo = (Mass_evoparated(i)*x5*Psat5*296.48794)/(x1*Psat1*170.34 + x2*Psat2*198.394+ x3*Psat3*46.06844+ x4*Psat4*282.46136+ x5*Psat5*296.48794);

end

Mass_dodecane_left = Mass_dodecane_initial - Mass_evoparated_dodecane;

Mass_tetradecane_left = Mass_tetradecane_initial - Mass_evoparated_tetradecane;

Mass_ethanol_left = Mass_ethanol_initial - Mass_evoparated_ethanol;

Mass_oa_left = Mass_oa_initial - Mass_evoparated_oa;

Mass_mo_left = Mass_mo_initial - Mass_evoparated_mo;

 $x1(i) = (Mass_dodecane_left/170.34)/(Mass_dodecane_left/170.34 + Mass_tetradecane_left/198.394 + Mass_ethanol_left/46.06844 + Mass_oa_left/282.46136 + Mass_mo_left/296.48794);$

 $x2(i) = (Mass_tetradecane_left/198.394)/(Mass_dodecane_left/170.34 + Mass_tetradecane_left/198.394 + Mass_ethanol_left/46.06844 + Mass_oa_left/282.46136 + Mass_mo_left/296.48794);$

 $x3(i) = (Mass_ethanol_left/46.06844)/(Mass_dodecane_left/170.34 + Mass_tetradecane_left/198.394 + Mass_ethanol_left/46.06844 + Mass_oa_left/282.46136 + Mass_mo_left/296.48794);$

 $x4(i) = (Mass_oa_left/282.46136)/(Mass_dodecane_left/170.34 + Mass_tetradecane_left/198.394 + Mass_ethanol_left/46.06844 + Mass_oa_left/282.46136 + Mass_mo_left/296.48794);$

 $x5(i) = (Mass_mo_left/296.48794) / (Mass_dodecane_left/170.34 + Mass_tetradecane_left/198.394 + Mass_ethanol_left/46.06844 + Mass_oa_left/282.46136 + Mass_mo_left/296.48794);$

end

[A.2] Properties

Temperature independent properties of the components:

1) Normal boiling Point:

Do-decane = 490 K

Tetra-decane = 526K

E than ol = 351 K

Methyl Oleate = 617K

 Molecular weights: (g/mole)

> Do-decane = 170.33 Tetra-decane = 198.388 Ethanol = 46.06884 Methyl Oleate = 296.487

Temperature dependent properties of components used:

(i) Density

$$\mathbf{D} = \frac{A}{B^{n}\left[1 + \left(1 - \frac{T}{C}\right)^{D}\right]}$$

The constants A,B,C and D are as follows:

For Dodecane:	For Tetra-decane	For ethanol	For Methyl Oleate
A = 0.33267	A = 0.27248	A = 1.6288	A = 0.24755
B = 0.24664	B = 0.24007	B .= 0.27469	B = 0.2624
C .= 658	C = 693	C = 514	C = 764
D = 0.28571	D = 0.28571	D = 0.23178	D = 0.33247

(ii) Enthalpy of vaporization:

 $\mathbf{Y} = \mathbf{A} \, (1 \text{-} T_r) (B + C T_r + D T_r^2)$

For Dodecane:	For Tetra-decane	For ethanol	For Methyl Oleate
A = 109620000	A = 120070000	A = 65831000	A = 213770000
B = 1.5544	B = 1.445	B = 1.1905	B = 2.3882
C = -1.5358	C = -1.3846	C = -1.7666	C = -2.873
D = 0.46286	D = 0.42836	D = 1.0012	D = 1.0193

(iii) Heat Capacity of gas:

$$Y = A + B \left[\frac{\frac{c}{T}}{\sinh\left(\frac{c}{T}\right)}\right]^2 + D \left[\frac{\frac{E}{T}}{\cosh\left(\frac{E}{T}\right)}\right]^2$$

For Dodecane:	For Tetra-decane	For ethanol	For Methyl Oleate
A = 212950	A = 230820	A = 49200	A = 329970
B = 663300	B = 786780	B .= 145770	B = 971600
C = 1715.5	C = 1682.3	C = 1662.8	C = 1645.6
D .= 451610	D = 544860	D = 93900	D = 674480
E .= 777.5	E.= 743.1	E .= 744.7	E.= 748

(iv) Heat capacity of liquid:

 $\mathbf{Y} = \mathbf{A} + \mathbf{B}\mathbf{T} + \mathbf{C}T^2$

For Dodecane:	For Tetra-decane	For ethanol	For Methyl Oleate
A = 508210	A = 353140	A = 102640	A = 324000
B = -1368.7	B = 29.13	B .= -139.63	B = 928
C = 3.1015	C = 0.86116	C = -0.030341	$\mathbf{C} = 0$

(v) Thermal Conductivity of liquid:

Y = A + BT

For Dodecane:	For Tetra-decane	For ethanol	For Methyl Oleate
A = 0.2047	A = 0.20293	A = 0.2468	A = 0.27248
B = -0.0002326	B = -0.00021798	B .= -0.000264	B = -0.000142

(vi) Vapour Pressure of Liquid:

 $\mathbf{Y} = e^{A + \frac{B}{T} + Cln(T) + DT^E}$

For Dodecane:	For Tetra-decane	For ethanol	For Methyl Oleate
A = 137.47	A = 140.47	A = 73.304	A = 187.49
B = -11976	B = -13231	B .= -7122.3	B = -19153
C = -16.698	C = -16.859	C = -7.1424	C = -22.989
D .= 0.0000080906	D = 0.0000065877	D = 0.000028853	D = 0.0000072769
E .= 2	E.= 2	E .= 2	E.= 2