

## **Numerical Investigation of Evaporation Modelling for Different Diesel Fuels at High Temperature and Pressure in Diesel Engine**

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Ali Raza \*, Sajjad Miran \*\*, Tayyab Ul Islam\*, Muhammad Khurram\*, Marva Hadia \*\*\*

\*Department of Mechanical Engineering, National University of Technology, IJP Road Islamabad, 44000, Pakistan.

\*\*Department of Mechanical Engineering, University of Gujrat, Gujrat 50700, Pakistan

\*\*\*Department of Mechanical Engineering, School of Mechanical and Manufacturing Engineering, National University of Sciences and Technology, Islamabad, 44000, Pakistan.

\* Corresponding Author: [muhammadkhurram@nutech.edu.pk](mailto:muhammadkhurram@nutech.edu.pk)

### **ABSTRACT**

Diesel engines are used widely in the world due to their capability of handling high torque and heavy loads efficiently. Fuel injection systems in the diesel engine have different processes that affect the complete burning of fuel in the combustion chamber. These include the primary and secondary breakup of liquid fuel droplets and evaporation. Diesel engines use the air as a working substance only. One of the processes is the evaporation of fuel droplets. Complete evaporation of diesel fuel liquid in the combustion chamber is a prerequisite for complete combustion. Hence evaporation of droplets has an impact on the efficiency of the engine and consequently on the output power and torque. In the present paper evaporation of two different diesel fuels is modeled numerically taking into account the turbulence effects present in the cylinder due to high temperature and pressure using the RANS turbulence model. Evaporation of n-heptane diesel fuel and n-decane is controlled by the numerical model that includes the conservation equations of mass, energy, momentum and species transport. During the evaporation phase heat is transferred to the droplet and due to evaporation from the surface of the droplet, the mass of evaporating droplets is decreased. These two processes are controlled by the equations of the Discrete Phase Model present in the Fluent. Then the results are plotted by varying the droplet diameter and temperature. Results include the decay in droplet diameter, increase in the droplet temperature effect on the velocity of droplet and temperature changes in the

cylinder due to evaporation of fuel. There are different parameters which affect the rate of evaporation of fuel droplets inside the engine cylinder of an internal combustion engine. These parameters include the diameter of fuel droplets, initial temperature of fuel droplets, and the temperature inside the cylinder after the compression stroke and surface area of droplets. Small droplets need a short time to evaporate while if the size of droplets is large then evaporation times is also increased.

**Keywords:** Droplet Evaporation; RANS; Turbulence; Diesel Fuel; Combustion; Numerical Analysis.

## INTRODUCTION

Automotive industries aim to enhance the efficiency and power output of engines remaining in the range of imposed standard emission principles which are becoming strict and rigorous day by day (Heywood, J. B. et al. 2018; Stone, R. et al. 1999). There are various in-cylinder processes that control the output power and efficiency of engines that including preparation of air-fuel mixture, spray breakup, evaporation, and combustion. Complete vaporization of fuel is necessary in the combustion chamber for complete combustion. Combustion and evaporation directly affect the efficiency and output power of an engine. (Perrin, H. et al. 2010; Walter, B. et al. 2010). Amongst the above-mentioned processes evaporation of fuel spray is an important phenomenon that directly affects the emissions and efficiency of engine. The complete evaporation of the diesel fuel droplets before combustion is a prerequisite to the efficient burning of fuel (Curtis, E et al. 1995). In industrial and commercial applications the importance of accurate modeling of evaporation of fuel spray droplets in the engine cylinder is known well (Chin, J. S. et al., 1983, Lefebvre, A. H. et al., 2017). Vaporization of diesel fuel droplets has been modelled numerically and experimentally in a broad way in the recent decades because of its applications in the wide range of engineering purposes (Ra, Y. et al., 2009; Brenn, G. et al. 2007; Tamim, J. et al., 1995). Evaporation modelling of diesel fuel droplets was started by

Landis and Mills (Landis, R. B. et al., 1974) followed by Law (Law, C. K. et al. 1982). In (Tamim, J. et al., 1995) evaporation of heptane-octane droplets is studied. Evaporation of diesel fuel droplets in internal combustion engines takes place at high temperatures and pressure. Fuel is injected in form of spray from the nozzle hole at a temperature higher than the saturation temperature of fuel. In this way fuel becomes superheated and its temperature is above the critical value (Prausnitz, J. et al. 1998, Bellan, and J. et al.). Many researchers have studied the evaporation of fuel droplets in these supercritical conditions. During the evaporation process, gas phase is governed by the Eulerian approach while droplet trajectories are traced in a Lagrangian frame (Gosman, A. D. et al., 1983). In the present work equations of energy, mass, momentum, and species are coupled and numerically solved to model the overall evaporation of two different diesel fuels. Evaporation of diesel fuel droplets present in the combustion chamber starts from surface diffusion. Molecules on the surface of droplets diffuse into hot air present in the combustion chamber. Rate of evaporation of droplets depends upon the diffusion of molecules from droplet surface into hot air evaporation and combustion. Amongst the above mentioned processes evaporation of fuel spray is an important phenomenon that directly affects the emissions and efficiency of engine. The complete evaporation of fuel droplets before combustion is a prerequisite for efficient burning of fuel (Ra, Y. et al., & Reitz, R. D. et al. 2009). In industrial and commercial applications the importance of accurate modelling of evaporation of fuel spray droplets in the engine cylinder is known well. Vaporization of diesel fuel droplets has been modelled numerically and experimentally in a broad way in the recent decades because of its applications in the wide evaporation of heptane-octane droplet is studied. Evaporation of diesel fuel droplets in an internal combustion engines takes place at high temperature and pressure. Fuel is injected in form of spray from fuels. Evaporation of the diesel fuel droplets present inside the combustion chamber starts from surface diffusion. Molecules on the surface of droplet diffuse into hot air present in the combustion chamber. Rate of evaporation of droplets depends upon the diffusion of molecules from droplet surface into hot

air environment (Abramzon, B. et al., 1989;). Evaporation process of liquid fuel droplets is completed into two parts. First one is the detachment of molecules and second is diffusion of vapors in the hot air (Haider, A. et al., 1989). In the present work a discrete phase model (DPM) is used to evaporate the different diesel fuels in the combustion chamber. There are two steps in the DPM calculation. First it solves the continuous phase present in the chamber that is air and then it solves the discrete phase followed by the continuous phase (Raza, A., Mehboob et al. 2020). Droplets are injected the in the engine cylinder by creating a discrete phase injection. There are different types of injections that can be applied. In this work single injection is used to inject the liquid fuel in the chamber. Unsteady particle tracking is done through the DPM in the continuous phase. Liquid particles are injected in form of spray from hole that disperse in the continuous phase. Particle trajectories are also observed in the continuous phase at high temperature and pressure in Lagrangian frame of reference. At high operating conditions inside the combustion chamber, high turbulence is induced during the spray breakup and evaporation process. To account for these turbulence effects RANS turbulence model is implemented in the evaporation model. A two equations realizable k-e turbulence model is used here. The above mentioned model is simple to implement and is inexpensive computationally. This model predicts the behavior of planar jets in an accurate way and takes into account the effects of fully turbulent flows. The evaporation process is implemented in the Ansys Fluent using discrete phase model coupled with species transport and RANS turbulence model.

## **GOVERNING EQUATIONS**

Generally, vaporization of diesel fuel droplets is controlled by continuity equation following the momentum, energy and species transport equation in numerical modelling. Continuity equation is used to conserve the mass of liquid fuel droplets. In the evaporation process mass conservation phenomenon is controlled by the continuity equation. Droplet has some velocity

when it comes out of the nozzle. Therefore, momentum equations is applied for the conservation of momentum. This momentum equation involves the pressure, gravity, and stress terms. Energy equation is also coupled with all these equation due to sensible enthalpy of droplet. Heat added to the liquid mass of the fuel is not used directly to evaporate the fuel droplets but initially fuel droplet is heated and then evaporation starts. Due to this heat up period heat energy is absorbed by the droplet and heat transfer equations comes into play for the fuel droplets. Heat transfer from ambient to the droplet depends upon the temperature inside the engine cylinder after compression stroke and is proportional to the droplet surface area. It is also linked with the initial droplet temperature. Finally, turbulence generated in the cylinder is taken into account using the RANS model. There are different turbulence models available in Ansys Fluent that includes RANS and LES. In the current study a Realizable k-e model is used. LES becomes computationally expensive as compared to RANS. For the current work RANS is acceptable.

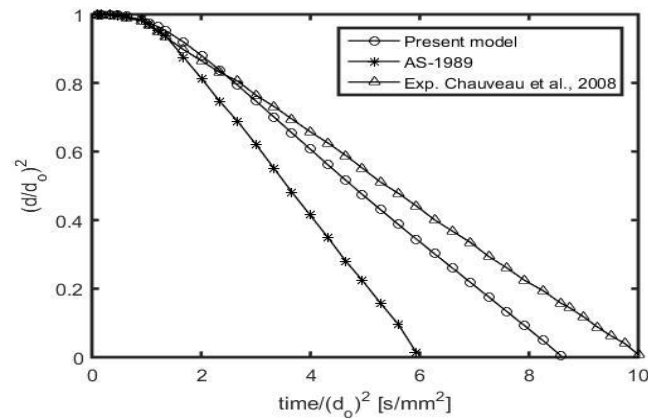
### **NUMERICAL MODELLING**

Ansys Fluent is used to apply the discrete phase model to the vaporization process of both n-heptane and n-decane fuels inside the combustion chamber at high temperature and pressure conditions in the presence of turbulence. Presence of turbulence is proved by the Reynolds number around the droplet. Governing equations used to control the evaporation process of fuel droplets include the mass, energy and momentum equations. To account for the turbulence effects a turbulence model is also necessary to couple with these conservations equations. Therefore, a RANS turbulence model is applied to the current work. A Realizable k-e turbulence model is applied with the all other models. Heat transfer effects on the droplets are governed by the heat transfer equations that include the species diffusion equations. There are two phases present in the engine cylinder. Compressed air acts as a continuous phase and injected droplets acts as discrete phase. Droplets are injected into continuous phase and evaporations process is governed by the above presented numerical model.

The above presented numerical model is applied to the real engine having the following specifications. Bore and stroke of the engine are 150 mm and 180 mm respectively. Maximum torque and ambient pressure are 295 kg-m and 4 MPa. A six-hole nozzle is used for the purpose of injection with each hole having diameter of 0.29 mm. injection pressure is kept as 20 MPa. The exit velocity of droplet from nozzle hole is 35 m/s and initial temperature of droplet is 300 K.

### **MODEL VALIDATION**

Evaporation model for diesel fuel droplets given above is applied in Ansys Fluent. The result extracted from the numerical model are then compared with the most valid evaporation results by (Chauveau et al. 2008). Results obtained in the current numerical model are also close to the results presented in (Abramzon, B. et al., 1989) and also with the earlier work in (Raza, A., Mehboob et al. 2020). Results including droplet regression rate and increase in the temperature of droplet are close to the numerical results presented in (Ebrahimian Shiadeh, S. V. et al. 2011) at different temperatures. Comparison of droplet regression rate are plotted with the results of (Chauveau, C. et al., 2008) and (Abramzon, B. et al., 1989). In figure 1 results of present model for n-decane are compared with the experimental results of (Chauveau, C. et al., 2008) and numerical results of (Abramzon, B. et al., 1989). Obtained results are close to the experimental and numerical values. It is seen that current model of fuel droplet vaporization is close to the experimental work by (Chauveau, C. et al., 2008). The difference between the results of numerical model presented in current study and the numerical model given by (Abramzon, B. et al., 1989). Is due to the fact that in the current study a turbulence model is also applied to take into account the effects of high turbulence.



**Figure 1:** Comparison of Present model for n-decane droplet vaporization with the experiment of Chauveau et al. and Numerical results of AS-1989 at 623K

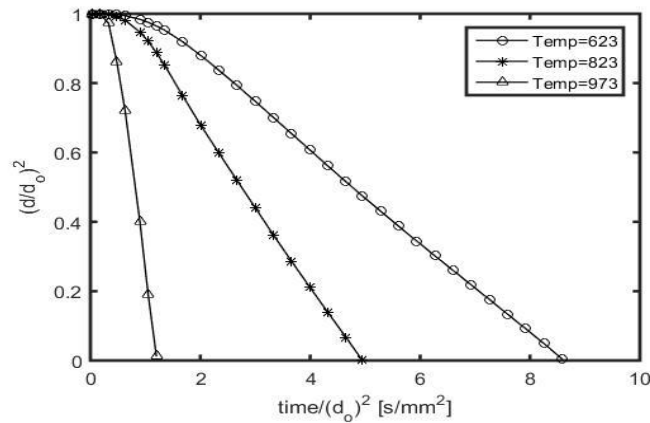
### Results Analysis

In the following section results for n-decane and n-heptane fuel droplets are presented at different ambient conditions. Normalized droplet diameters are plotted using D-square law against the normalized time. Two different sizes of droplets are considered to note the outcome of changes in the ambient temperature of engine cylinder. Increase in droplet temperature is plotted with respect to the injection duration. It is seen that droplets which have same size do not evaporate in a same manner at different conditions i.e. at different temperatures.

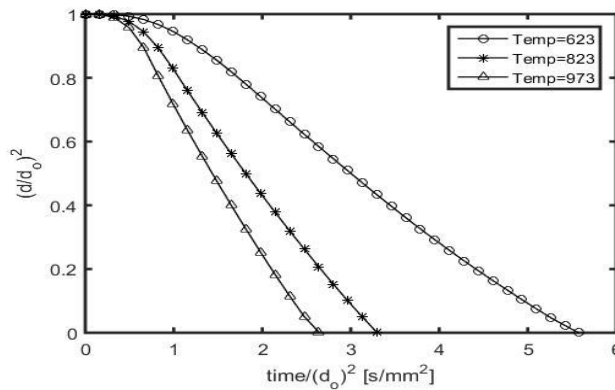
#### Case 1 fuel n-decane

In figure 2 it is clear that n-decane droplet of 10-micron diameter evaporates completely in a short period of time at high ambient temperature of 973K as compared to the other lower ambient temperatures of 623K and 823K. Similarly, in figure 3 vaporization of n-decane droplets of the 20 micron is plotted and a same trend is observed again. It has been observed that if the size of the droplets is same then their evaporation rate is directly proportional to the ambient temperature. As the ambient temperature increased evaporation rate is also increased. As the ambient temperature decreased evaporation rate is also decreased. Fuel is sprayed in the combustion chamber in form of fine droplets. After atomization fuel break ups into primary and

secondary break up. After these fuel droplets travels along the combustion chamber. When fuel is atomized, droplets face the drag force and turbulence induced in the cylinder due to high temperature and pressure conditions. Due to this fact velocity of droplet is decreased. Velocity is also decreased due to the reduction in mass of droplet. Velocity of large droplets takes more time to reach minimum value and vice versa.



**Figure 2:** Vapourization of 10 micron n-decane droplet for different temperatures



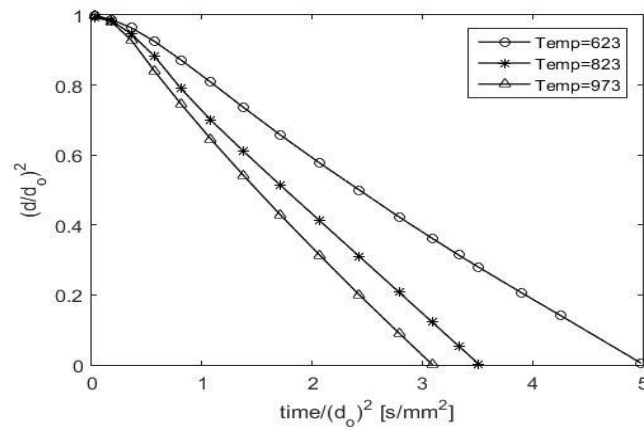
**Figure 3:** Vapourization of 20-micron n-decane droplet for different temperatures

### Case 2 fuel n-heptane

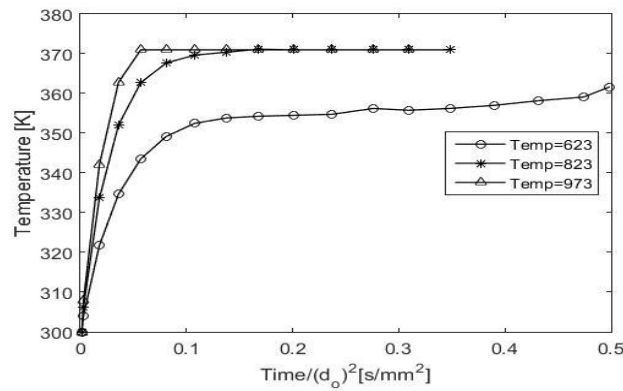
In this section droplets of sizes 10 and 20 microns are considered. It is noted that if the size of droplets is small then the evaporation time is also small. Temperature inside the engine cylinder have also impact on the evaporation of diesel fuel droplets. It is clear that if the temperature is high evaporation rate is also high and if the ambient temperature is low evaporation rate is also



low. At temperature of 973K the droplet life time is much shorter than the temperature of 623K. Also it is observed that evaporation time of n-heptane fuel droplets is lower than the n-decane. In figure 4 regression in diameter of n-heptane fuel droplet of size 10 micron is plotted using  $D^2$ -law with the normalized evaporation time. It is obvious that at lower ambient temperature of 623K droplet life is higher than the temperatures of 823 and 973k. At lower temperature of 623K evaporation of time is almost 45 % greater than the temperature at 823K. While at a higher temperature of 973K evaporation time and droplet life is much short as compared to the other two cases. In figure 5 Temperature profiles of n-heptane 10-micron droplet is plotted with the normalized droplet evaporation rate and a same trend can be seen as in case of droplet regression with time. At higher temperature of 973K droplet lifetime is much short than the 623K. For the temperature of 623K droplet residence time is more than the temperatures of 823K and 973K. In figure 6 evaporation of 20 micron droplet is plotted against the normalized time. In this figure it can be seen clearly that by increasing the size of size of droplet evaporation time of droplet also increased. In figure 6 regression rate of a 20-micron diesel fuel droplet is plotted at various ambient temperatures. Evaporation time of fuel droplets at high ambient temperature is low and vice versa. In figure 7 gain in temperature of 20-micron droplet are plotted with the time. For low ambient temperatures droplets having large size take more time for complete evaporation. It is evident that as the droplet size is increased heat up period, droplet lifetime and evaporation time is increased at the same ambient temperatures. In figures below it can be seen that when size of droplet is increased droplet lifetime is increased appreciably. It is due to the fact that when size is increased mass is also increased. Evaporation starts from the surface and it is a surface phenomenon. Due to increases mass and surface area heat up period is also increased and eventually droplet life time and evaporation time is also increased.

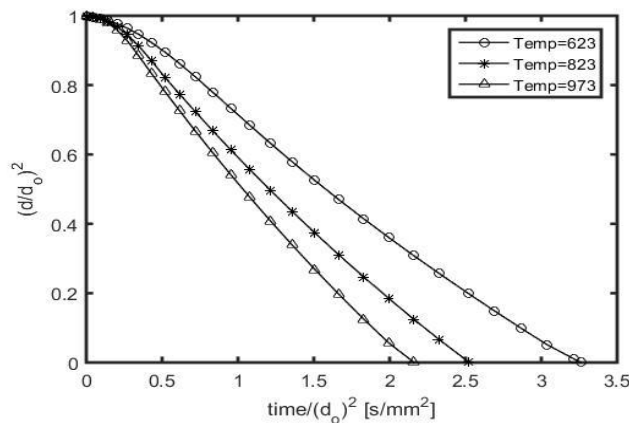


**Figure 4:** Vaporization of 10 micron n-heptane droplet for different temperatures

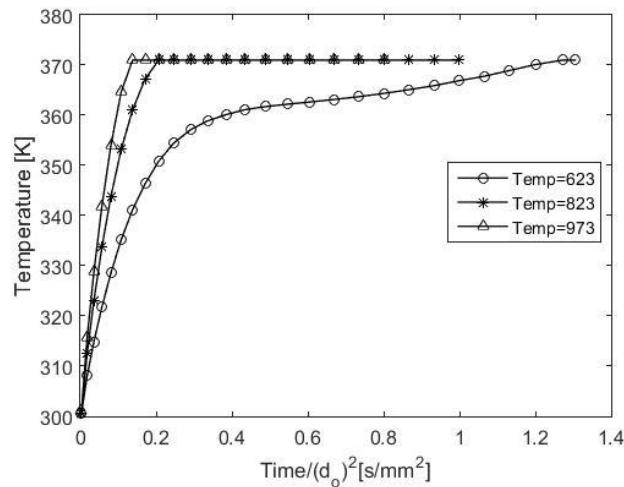


**Figure 5:** Droplet Temperature of 10 micron

Contours of the droplet mass fraction and temperature of the droplet inside the 1/6<sup>th</sup> sector of combustion chamber are shown here for n-decane droplet of 10 microns. Nozzle has six holes which ejects the 6 jets in six sectors of engine cylinder 60 degrees apart from each other. In the figures below mass fraction contours are shown at various planes and axis.

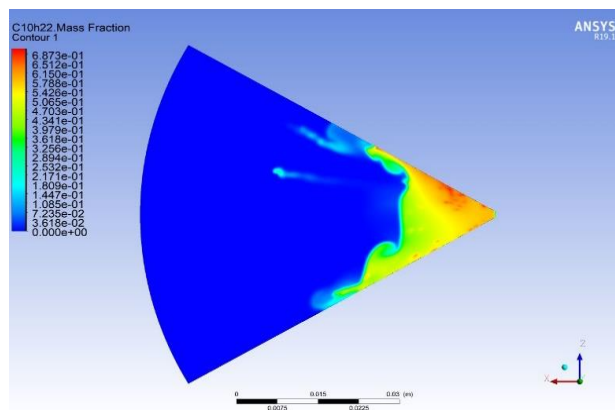


**Figure 6:** Vaporization of 20 micron n-heptane droplet for different temperatures



**Figure7:** Droplet Temperature of 20 micron

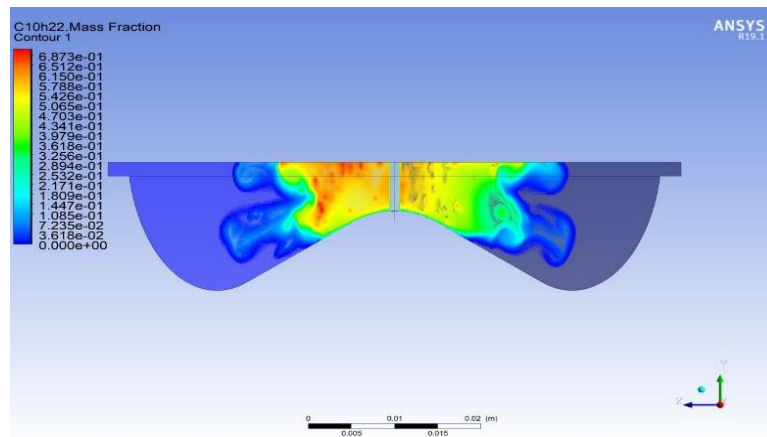
In figure 8 a top view of 1/6<sup>th</sup> portion of one sixth sector of combustion chamber is shown. In this view it is shown that when jet is evolved from the nozzle it splits approximately equally in the two sides of chamber sector. It is due to the fact that cone angle of 30 degrees is kept for the injection. This one sixth sector has total 60 degrees angle due to the fact that cylinder is divided into 6 sector and each has 60 degrees total angle. When jet is evolved from the nozzle hole it splits into two streams and equal amount of mass is distributed.



**Figure 8:** Contours of mass fraction of n-decane 10 micron droplet

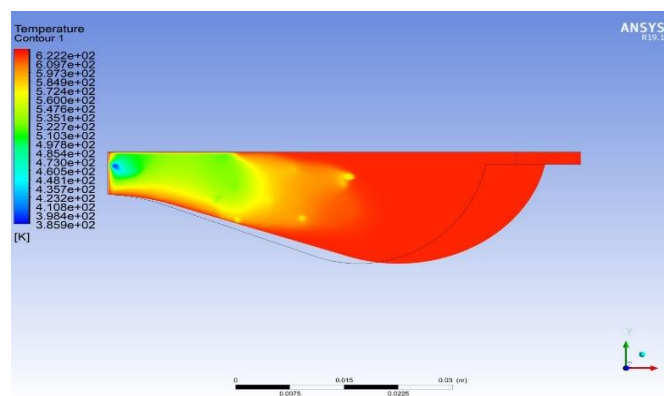
It is seen in figure 9 that jet is not struck to the side wall of sector rather it is vanished before the half of the length from the center to the wall. Blue area in the contours show that there is zero mass fraction there. Yellow color in contours is dominant on both sides that shows the

uniformity. Mass fraction contours show that all the mass injected in form of droplets is vaporized in the sector of engine cylinder.



**Figure 9:** Contours of mass fraction of n-decane 10 micron droplet

Similarly figure 10 shows the temperature contour of one sixth sector of engine cylinder. It can be seen that where droplets are present the temperature is lower than the rest area. Initial ambient temperature of engine cylinder was 623K but after injection temperature at the place where injected particles travelled is lower down due to the evaporation of fuel droplets. In figure 10 plane contour is shown for temperature. It shows the temperature of sector in the presence of fuel mass fraction. Maximum temperature is 623K and minimum is 385K of the sector.



**Figure 10:** Contours of Temperature of n-decane 10 micron droplet

The present evaporation model works for the real engine applications. But certain things need to be addressed. Droplet diameter should be as small as possible to evaporate the mass quickly.

In this work it is recommended that nozzle hole size should be designed in a way so that after break up and other effects including the penetration length final size should reach up to 10 micron. In this study three different diameters are taken to see the evaporation time and droplet life time. It is obvious that droplets of small diameters evaporate more quickly. Nozzle hole taken in this study has a diameter of 290 micron. If nozzle hole is reduced it will also affect the size of droplet after penetration length and average diameter can be obtained smaller. Also a large amount of droplets is gathered inside the engine cylinder and not necessarily every droplet evaporates completely. Some droplets strike the head wall before the complete evaporation. If diameter is as small that they do not strike the wall and evaporate completely before striking the wall it will produce more efficient combustion and hence increased efficiency can be achieved.

### **CONCLUSION**

In this research evaporation of liquid fuel droplets of n-heptane and n-decane fuels is modelled numerically by considering the effects of turbulence present inside the combustion cylinder because of high temperature and pressure using Realizable k-epsilon turbulence model. Results show that droplet having the large size need more time for complete evaporation and droplets having small size need less time for the same. Heat up period of small droplets is also short and due to this fact they evaporate in a short period of time. Droplets of same size show different behavior at different ambient temperatures. Droplet evaporation time for high temperature is less than the low temperature. Further temperature histories of fuel droplets are plotted with the injection time that shows that small droplets evaporate quickly by absorbing the temperature quickly. Droplets having larger diameters sustain for more time and their evaporation time is greater. Velocity of droplet is also plotted with the injection time and this is confirmed that at the same velocity, the diesel fuel droplets of small diameters have short heat up period and hence short evaporation time than the large size droplets. In the end comparison for both fuels is also given at same operating conditions and it is observed that n-heptane fuel droplets

evaporate in a short time than the droplets of n-decane fuel droplets.

## REFERENCES

- Heywood, J. B. (2018).** *Internal combustion engine fundamentals*. McGraw-Hill Education.
- Stone, R. (1999).** *Introduction to internal combustion engines* (Vol. 3). London: Macmillan.
- Perrin, H., Dumas, J. P., Laget, O., & Walter, B. (2010).** Analysis of combustion process in cold operation with a low compression ratio diesel engine. *SAE International Journal of Engines*, 3(1), 1012-1032.
- Walter, B., Perrin, H., Dumas, J. P., & Laget, O. (2010).** Cold operation with optical and numerical investigations on a low compression ratio diesel engine. *SAE International Journal of Engines*, 2(2), 186-204.
- Curtis, E. W., Uludogan, A., & Reitz, R. D. (1995).** A new high pressure droplet vaporization model for diesel engine modeling. *SAE paper*, 952431.
- Chin, J. S., & Lefebvre, A. H. (1983).** Steady-state evaporation characteristics of hydrocarbon fuel drops. *AIAA journal*, 21(10), 1437-1443.
- Lefebvre, A. H., & McDonell, V. G. (2017).** *Atomization and sprays*. CRC press.
- Ra, Y., & Reitz, R. D. (2009).** A vaporization model for discrete multi-component fuel sprays. *International Journal of Multiphase Flow*, 35(2), 101-117.
- Brenn, G., Deviprasath, L. J., Durst, F., & Fink, C. (2007).** Evaporation of acoustically levitated multi-component liquid droplets. *International journal of heat and mass transfer*, 50(25-26), 5073-5086.
- Tamim, J., & Hallett, W. L. (1995).** A continuous thermodynamics model for multicomponent droplet vaporization. *Chemical Engineering Science*, 50(18), 2933-2942.
- Landis, R. B., & Mills, A. F. (1974).** Effect of internal diffusional resistance on the evaporation of binary droplets. In *International Heat Transfer Conference Digital Library*. Begel House Inc.
- Law, C. K. (1982).** Recent advances in droplet vaporization and combustion. *Progress in energy and combustion science*, 8(3), 171-201.
- Prausnitz, J. M., Lichtenthaler, R. N., & De Azevedo, E. G. (1998).** *Molecular thermodynamics of fluid-phase equilibria*. Pearson Education.
- Bellan, J. (2000).** Supercritical (and subcritical) fluid behavior and modeling: drops, streams, shear and mixing layers, jets and sprays. *Progress in energy and combustion science*, 26(4-6), 329-366.
- Gosman, A. D., & Loannides, E. (1983).** Aspects of computer simulation of liquid-fueled combustors. *Journal of energy*, 7(6), 482-490.

**Ra, Y., & Reitz, R. D. (2009).** A vaporization model for discrete multi-component fuel sprays. *International Journal of Multiphase Flow*, 35(2), 101-117.

**Abramzon, B., & Sirignano, W. A. (1989).** Droplet vaporization model for spray combustion calculations. *International journal of heat and mass transfer*, 32(9), 1605-1618.

**Haider, A., & Levenspiel, O. (1989).** Drag coefficient and terminal velocity of spherical and nonspherical particles. *Powder technology*, 58(1), 63-70.

**Chauveau, C., Halter, F., Lalonde, A., & Gökalp, I. (2008).** An experimental study on the droplet vaporization: effects of heat conduction through the support fiber. In *22 nd Annual Conference on Liquid Atomization and Spray Systems (ILASS Europe 2008)*.

**Ebrahimian Shiadeh, S. V. (2011).** *Development of multi-component evaporation models and 3D modeling of NOx-SCR reduction system* (Doctoral dissertation).

**Raza, A., Mehboob, H., Miran, S., Arif, W., & Rizvi, S. F. J. (2020).** Investigation on the Characteristics of Biodiesel Droplets in the Engine Cylinder. *Energies*, 13(14), 3637.