Droplet Evaporation and Ignition at High Pressure

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Abstract: The present work is a mathematical model for the droplet evaporation and ignition of a single droplet of a pure hydrocarbon fuel at high pressure. The finite difference method is used to solve transient equations of continuity, species and energy in the vapor phase and species and energy in liquid phase. The vapor-liquid equilibrium has been described by Peng-Robinson equation of state. In this model, the high pressure transient effects, variable thermo-physical properties and inert species solubility in the liquid-phase are considered. The evaporation model has been extensively validated with experimental results available in literature. The ignition model has been tested for ambient temperature of **1200 K**. The ambient pressure varies in the rage from **10 bar** to **80 bar**. The ignition delay was found to be strong functions of temperature, pressure and diameter. The ignition time decreases monotonically with increase in ambient pressure and temperature. At each pressure there existed a minimum diameter below which ignition does not takes place and this minimum diameter decreases with increase in pressure.

Keyward: **Droplet, evaporation, ignition, pressure**

I. INTRODUCTION

Droplet vaporization and ignition at high pressure is of great importance in the development of high pressure combustion systems such as diesel engines, gas turbines etc. The physical mechanisms occurring under high pressure conditions are different from that of low pressure conditions. Thus the conventional low pressure theories are not able to describe the high pressure characteristics. In diesel engines, gas turbines, rockets etc. the fuel is atomized to tiny droplets to enlarge the surface area for fast evaporation and ignition. The engine performance is highly dependent on the droplet vaporization and ignition process.

In order to have a better understanding of spray characteristic, it is essential to study the behavior of a single static droplet of fuel exposed to high temperature and pressure. As the droplet is heated by the ambient gas, first the difference in densities of gas and liquid phases becomes smaller. Thus, the transient effects in the gas phase are of same significance as those of liquid and the quasi-steady conditions are not attained during the lifetime of droplet. Secondly, the solubility of the ambient gas in the liquid phase increase with the increase in ambient pressure, thus the phase equilibrium analysis cannot be done by Rault's law. Third, at high ambient pressure increases, the latent heat decreases and the low pressure model will predict vaporization rate with errors. Attempts to study droplet vaporization and combustion under high ambient pressures have been made since last four decades. An excellent review of high pressure droplet evaporation and combustion has been given by Givler and Abraham [1].

The aim of present study is to develop a satisfactory model for droplet evaporation and ignition suitable for high temperatures and pressures. The model will include full transient effects and will take into account the non-ideal effects and absorption of surrounding gas in liquid. The model will also include pressure and temperature dependence of thermo-physical properties.

II. MODEL

The following assumptions are made to model the problem: Spherical symmetry and constant pressure, momentum equation is not solved in the gas phase as the pressure is assumed to be constant, Soret and Dufour effects are neglected, the radial velocity, which is non zero, has been evaluated from the continuity equation. The governing equations in the model are similar to that used by Kumar et. al [2]. Peng-Robinson's equation has been used at liquid-gas interface to incorporate real gas effects. Variable themo-physical properties from Reid et.al. [3] have been used to include the effects of high temperature and pressure.

(i)   Reaction rate model

The single step Arhenius type reaction rate model has been used for the droplet ignition. The values of kinetic parameters have been taken from Kumar et. al [2]. It has to be mentioned here that the effect of pressure on kinetic parameters have not been considered in the present work. This is primarily because adequate experimental data are not available. Also detailed reaction mechanism would have resulted in a very significant increase in computational time.

(ii)   Validation

The important aspect for droplet evaporation and ignition under high pressure conditions is solubility of surrounding gas in the droplet. The phase equilibrium results for n-heptane-nitrogen mixture were validated with the experimental data [4]. The model has also been validated with the experimental data of Nomura et al. [5] for a n-heptane droplet evaporating in nitrogen environment

for different ambient pressure were in good agreement with the experimental data. The detailed results of validation for phase equilibrium and droplet evaporation are given in [6].

III. RESULTS AND DISCUSSION

Results for high pressure combustion of n-heptane droplet are presented here. The droplet at $300\ K$ is introduced instantaneously into quiescent air whose temperature is set to $1200\ K$. Ambient pressure variation of $10-80\ bar$ for ignition characteristics and droplet size varying from $0.5-2.0\ mm$ has been considered. These parameters are typical of conditions in which droplets and sprays combustion takes place in a combustion chamber. Ignition of the droplet is said to occur if the temperature at ignition location exceeds from the surroundings by $100\ K$.

At high pressure as air gets absorbed in the liquid, the enthalpy change on evaporation is no longer that of pure liquid fuel. Figure (1) shows that enthalpy of evaporation decreases with increasing pressure and temperature and approaches zero at the critical point of the mixture. Similar, results have been shown by Hsieh and Sheun [7] and Kadota and Hiroyasu [8].
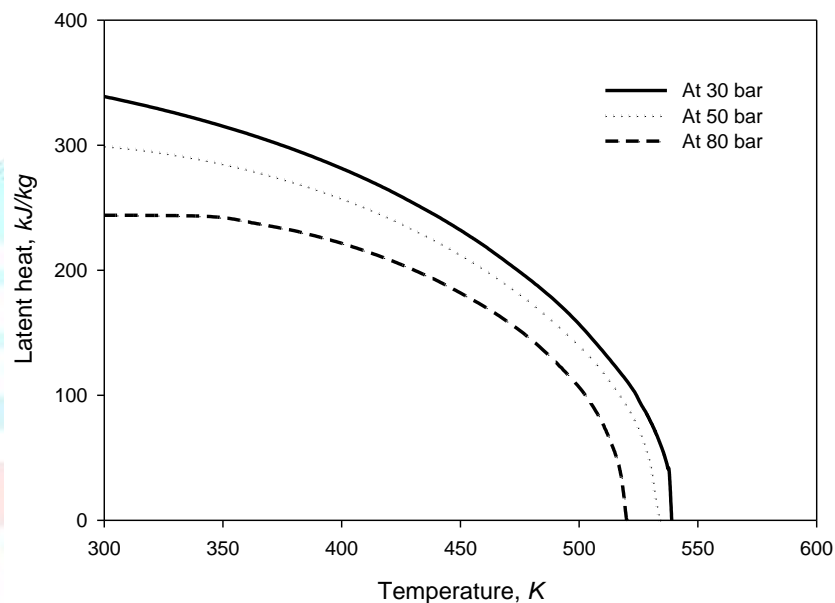

Figure: 1 Variation of enthalpy of evaporation with temperature at three different ambient pressure

Figure (2) shows that ignition time decreases sharply as ambient pressure rises, due to dependence on reaction rate. As the ambient pressure increases, the rate of vaporization actually decreases. As the ambient pressure rises, the partial pressure of fuel remains the same, so that the fuel mass fraction near the droplet surface decreases sharply thereby reducing the mass flux. The effect of reduced mass flux is to bring the reaction zone closer to the droplet surface and ignition occurs in progressively leaner mixtures as pressure rises. Despite leaner mixtures and progressively decreasing mass flux, the rapid ignition indicates that the reaction rate constants have much stronger dependence on pressure and temperature than on fuel concentration.
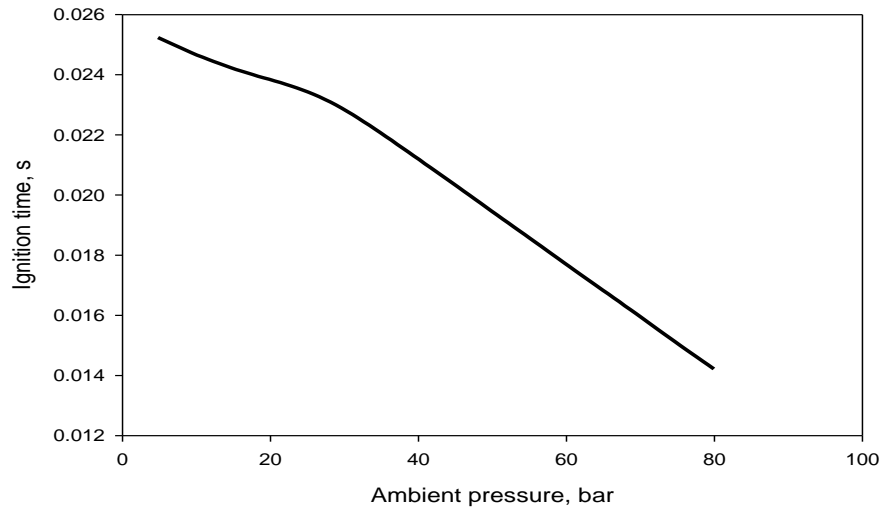
Figure: 2 Variation of Ignition time with ambient pressure at ignition for a droplet of initial diameter $0.5\ mm$.

Examination of predicted temperatures and fuel concentration profiles as shown in figure (3) – (5) showed that as pressure rises, the fuel mass fraction near the droplet surface decreases. This is to be expected, since the air partial pressure is rising while the fuel partial pressure remains largely unchanged. This leads to lower evaporation rates for droplets at higher pressures, which in turn means that more of the heat transferred to the droplet is used to heat the liquid. Hence, droplet heating is more rapid at high pressure. The results are presented in figure (3). Figure (4) and (5) shows that the concentration changes cause the reaction zone and the subsequent location of ignition to move closer to the droplet surface at high pressure. Reaction was found to take place under progressively leaner conditions as pressure rises..
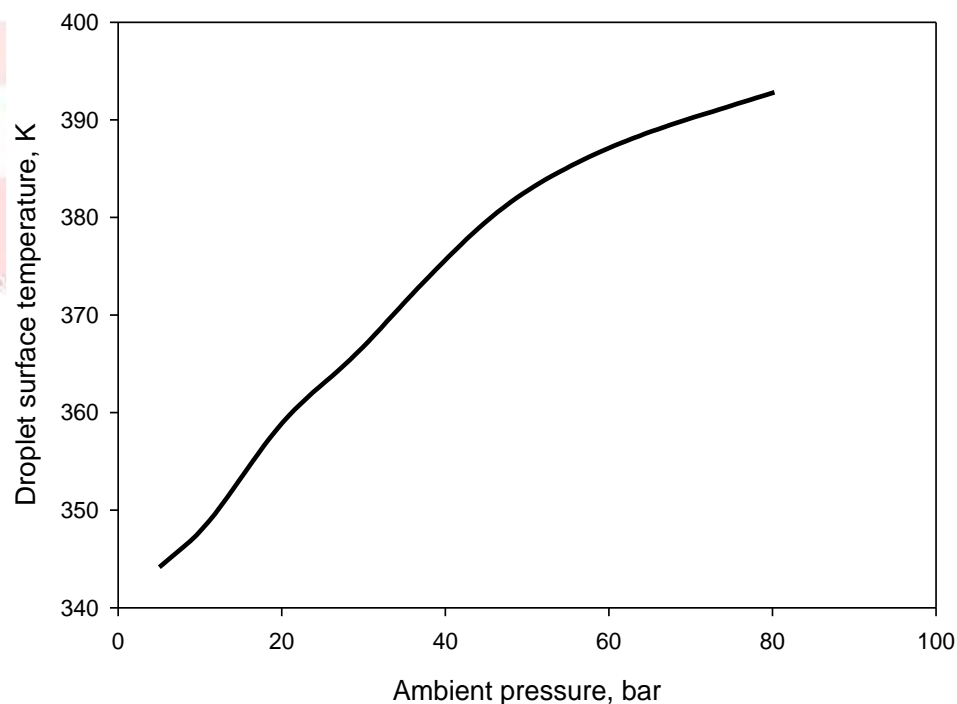
Figure: 3 Variation of droplet surface temperature with ambient pressure at ignition for a droplet of initial diameter $0.5\ mm$.
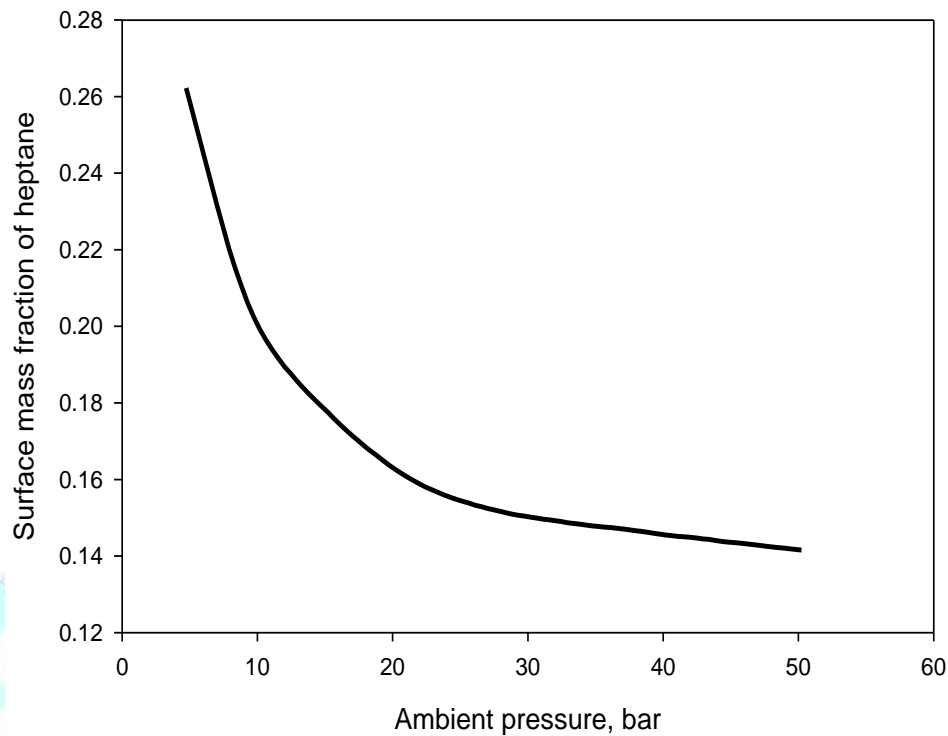
Figure: 4 Variation of gas side fuel surface mass fraction with ambient pressure at ignition for a droplet of initial diameter $0.5\ mm$.

Figure: 5 Variation of ignition location with ambient pressure at ignition for a droplet of initial diameter $0.5\ mm$.

Figure (6) shows the variation ignition time with droplet diameter at different ambient pressures. The pre-ignition time for large droplets is dominated by transient heating of the liquid and lead to a steeper variation of ignition time with diameter for this fuel. An increase in the initial temperature of the droplet diminishes the effect of transient heating, substantially reducing both ignition times and dependence on droplet diameter. Small droplets undergo rapid heating to high temperatures and produce large fuel vapor concentrations regardless of fuel boiling point.
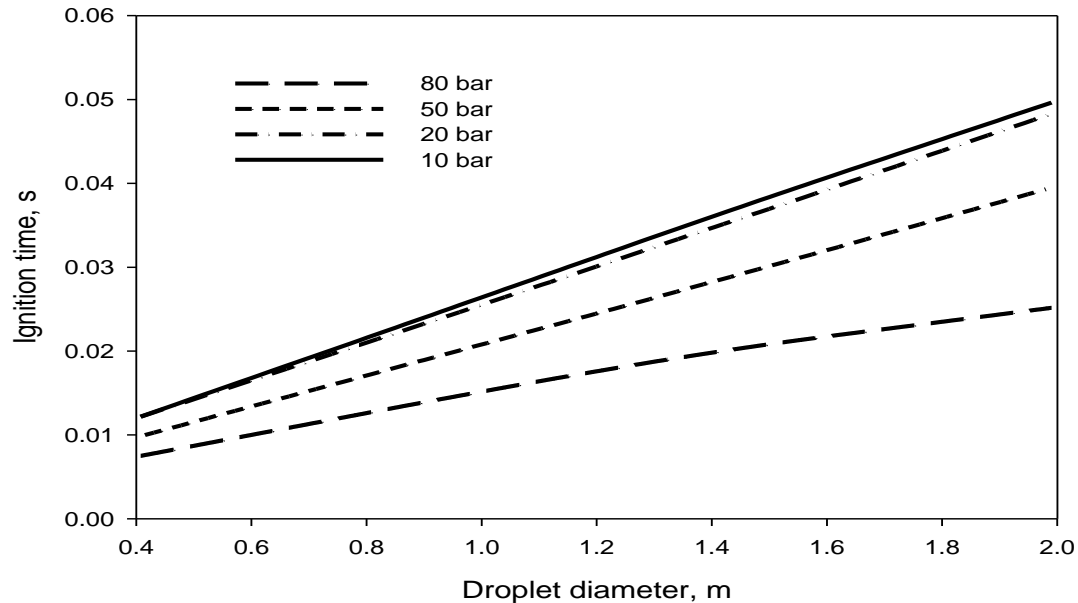
Figure: 6 Variation of ignition time with droplet diameter at different ambient pressures.

It is to be noted that the behavior of ignition delay with pressure depends strongly on the reaction orders i.e. exponents of fuel and oxygen concentration in the reaction rate expression in the model. In the present study, the values of exponents are those from the work of Kumar et.al [2] i.e., an exponent of $a = 1.0$ for fuel and $b = 1.0$ for oxygen. To find the effect of pressure on exponents a and b, it was decided to change the reaction constants to $a = 0.75, 1.25, 1.5$ for fuel and $b = 1.25, 0.75, 0.5$ for oxygen. The significance of $a = b = 1$ is that it was used by most ignition models in the past. Figure (7) shows the effect of changing these exponents. These changes have a significant effect on the reaction zone, which moves towards the droplet surface as a or b increases. Another result is a large change in delay time, evidence of a strong degree of control by chemical kinetics. It should be noted that overall pressure dependence of rate is given by $(a + b)$. Therefore, $a = 0.75, b = 1.25\ (a + b = 2)$ gives a steeper drop of ignition time with pressure than $a = 1.25, 1.5, b = 1.5\ (a + b = 2)$. However, $a = b = 1\ (a + b = 2)$ give a less steep dependence. The reason for this is that $a = 0.75, b = 1.25$ gives a much stronger effect of oxygen, hence ignition occurs more quickly. As compared to when the case $a = b = 1$.

An important topic in the literature on droplet behavior at high pressure has been the question of whether the liquid phase ever becomes supercritical. In the present work, since the ignition time becomes shorter as the pressure rises, ignition always occurs when the droplet is far short of critical state. Figure (3) shows that n-heptane droplets ignite at a liquid temperature below $400\ K$ regardless of pressure, while the critical temperature for pure n-heptane is $540\ K$.
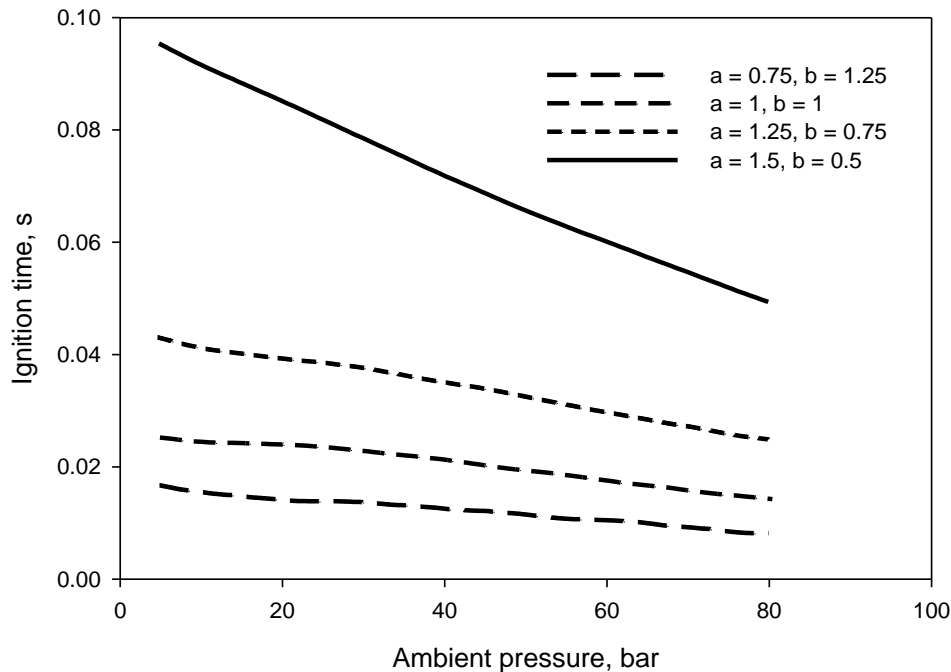
Figure: 7 Variation of ignition time with ambient pressure for different reaction exponents for a droplet with initial diameter of r = 0.5 mm,

IV CONCLUSIONS

The results of the mathematical model described show that the main effect of high ambient pressure and temperature is a substantial reduction in ignition delay time due to increase in the reaction rate which also causes the fuel to ignite even for leaner conditions. Ignition time increases with increase in droplet diameter at all the pressures. The reaction zone moves closer to the droplet surface as pressure rises.

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