Theoretical and Numerical Analysis of Fuel Droplet Vaporisation at high Temperatures

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Abstract:
In our work we present a theoretical analysis and numerical solution of fuels droplets vaporisation n-alkaline (n-heptane, n-octane, n-nonane and n-decane) that evaporate slowly in air to stagnant conditions, ambient temperature and pressure and at different temperatures. The results show that liquid fuel droplets which have the lowest molar mass vaporize quickly. Vaporisation rate becomes more significant when environment temperature increases. This is confirmed by the experimental results of M.Birouk (1996) and C.Morin (1999). Average and instantaneous vaporisation rates have been estimated from D^2 law at temperatures varying from 473 to 673 K and at atmospheric pressure.. The main objective of our study is to better understand the process of vaporizing droplets sprays, to better prepare the gas mixture in the combustion chambers and improve the combustion efficiency to reduce pollutant formation and of such as unburned carbon monoxide and NOx.

Key Words: droplets vaporisation, fuel droplet, droplets

Nomenclature

B	: Spalding number
B_M	: Mass transfer number
B_T	: Thermal transfer number
D	: Droplet diameter (m).
D_m	: Binary mass Diffusivity coefficient
Cp	: Specific heat (J/kg.K)
h	: Enthalpy (J/kg).
J	: Mass flux (kg/m^2 s).
K	: Vaporisation rate (m^2/s).
L_V	: Latent heat of vaporisation (J/kg).
L_{Ve}	: Effective latent heat of vaporisation (J/kg).
L_{Vteb}	: Latent heat of vaporisation at ebullition temperature (J/kg).
$\dot{m}$	: Mass flow rate (kg/s)
M	: Molecular Weight, kg/kgmol
M_a	: Air mass molar (kg).
M_F	: Fuel mass molar (kg).
Nu	: Nusselt number.
P	: Pressure (bar)
P_{Fs}	: Vapor pressure saturation (bar).
Pr	: Prandth number.

r	: Droplet radius (m).
S	: Surface (m^2).
t	: Times (s).
T	: Temperature (K).
Teb	: Ebullition temperature (K).
T_r	: Reference temperature (K)
T_S	: Surface temperature (K).
T_{Cr}	: Critic temperature point (K).
T_g	: Gas temperature (K).
Y	: Mass fraction.
Y_{ox}	: Mass fraction of air.
Y_F	: Mass fraction of fuel.

Greek symbols

Φ	: Heat transfer rate (W)
λ	: Thermal conductivity (W/ m.K)
ν	: Cinematic viscosity (m^2/s)
μ	: Dynamic viscosity (Kg/m.s).
ρ_L	: Droplet volume density (kg/m^3)
ρ_g	: Gas volume density (kg/m^3)

1. Introduction

Liquid droplet vaporisation in a high-temperature environment is of relevance to combustion science and technology such as liquid-propellant rockets, gas turbines, and diesel engines. In all these systems, liquid fuels and oxidizer are usually injected into the combustion chamber as a spray of droplets, which undergoes a sequence of vaporisation, ignition and combustion processes, at a high-temperature. The evaporation or simultaneous evaporation and combustion of a fuel droplet are frequently treated by using quasi-steady theories by Williams (1973) and Rosner (1972)), Frosling, 1938, Ranz and Marshall, 1952, Law and Williams 1972, Faeth 1977, Sato et al 1990. This article focuses on the study of spray droplets while we develop an algorithm that calculates the droplets fuel vaporisation rate in ambient conditions and different temperatures.

2. Mathematical model

The following assumptions are considered in the present model:
- The droplet is assumed to be spherical.
- The pressure is assumed to be constant and equal to the local mean ambient.
- No natural convection phenomena are present.
- Soret and Dufour effects are neglected.
- Equilibrium conditions at the droplet/gas interface are assumed.
- Uniform physical properties of the surrounding fluid.
- The gas phase Lewis number is assumed to be unity in the droplet mode
- Radiation between the droplets and their surroundings is neglected.

The governing equations are the usual conservation equations for species, energy and mass both for the gas and for the liquid phase.

2.1. Mass conservation

$$div(\rho.\vec{v}) = \frac{1}{r^2}\frac{d(r^2.\rho.v_r)}{d(r)} = 0 \qquad (1)$$

$$4.\pi.r^2\rho.v_r = \dot{m} \qquad (2)$$

2.2. Mass conservation for evaporation fuel

$$\dot{m}Y_F - 4\pi r^2 \rho_F D_m \frac{d(Y_F)}{dr} = ct_F \qquad (3)$$

2.3. Mass conservation for the oxidant

$$\dot{m}Y_{OX} - 4\pi r^2 \rho D_m \frac{d(Y_{OX})}{dr} = ct_{OX} \qquad (4)$$

The boundary conditions for the equations of mass, energy and species conservation are:

$$r = r_S \qquad T = T_S \qquad Y_F = Y_{Fs}$$
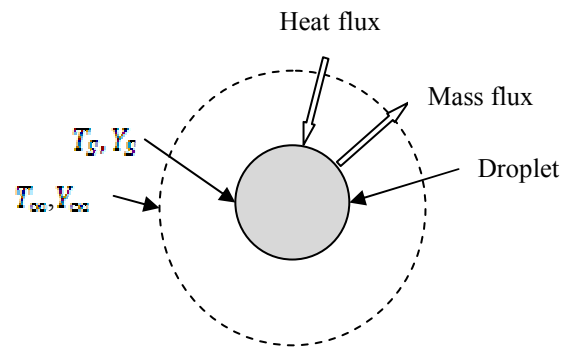$$r = \infty \qquad T = T_\infty \qquad Y_F = 0$$

Fig.1. droplet vaporisation processes

The profile of the fuel mass fraction and mass flow of spray can be written:

$$Y_F = 1 - \exp\left(-\frac{\dot{m}}{4\pi\rho_F D_m r}\right) \qquad (5)$$

$$\dot{m} = 4\pi\rho_F D_m r \ln(1 + B_M) \qquad (6)$$

Where

$$B_M = \frac{Y_{Fs}}{1 - Y_{Fs}} \qquad (7)$$

2.4. Energy conservation

$$div(\rho\vec{v}h) = div\left(\Phi + \sum_i h_i \vec{j_i}\right) \qquad (8)$$

Where

$$\Phi = -\lambda.\vec{grad}(T) \text{ (Fourier's law)} \qquad (9)$$

$$\vec{j_i} = -\rho D_i \vec{grad}(Y_i) \text{ (Fick's Law)} \qquad (10)$$

$$\dot{m}.T - 4.\pi.r^2.\rho.D_m.\frac{d(T)}{dr} = ct_T \qquad (11)$$

The conditions at the surface of the droplet give us:

$$T = T_S - \frac{Lv}{C_P} + (T_\infty - T_S + \frac{Lv}{C_P})\exp(-\frac{\dot{m}}{4\pi\rho_g D_m r}) \qquad (12)$$

$$\dot{m} = 4\pi\rho_g D_m r_g \ln(1 + B_T) \qquad (13)$$

Where

$$B_T = \frac{C_P(T_\infty - T_S)}{Lv_e} \qquad (14)$$

on taking into account the stationary system

$$B = B_M = B_T \qquad (15)$$

the expression of the change in squared diameter of the droplet during its evaporation as a function of time.

$$\frac{dD^2}{dt} = -8\frac{\rho_g}{\rho_L} D_m \ln(1+B) \qquad (16)$$

Where

$$K = -8\frac{\rho_g}{\rho_L} D_m \ln(1+B) \qquad (17)$$

In the quasi-steady theory the mass transfer number B_M and the thermal transfer number B_T are equal. This equality is used to determine by iteration the values of the droplet surface temperature and the mass fraction, required for the calculation of the theoretical vaporisation rate. To calculate the droplet surface temperature we have should followed the method that is adopted by Lefebvre (1989), this method is based to determine the two adimensional Spalding numbers B_M and B_T using the quasi-steady theory.

$$Y_{Fs} = \frac{1}{1 + \left(\frac{p_{amb}}{p_{Fs}} - 1\right)\left(\frac{M_a}{M_F}\right)} \qquad (18)$$

Where

M_a : is the air mass molar.

M_F : is the fuel mass molar.

p_{amb} : is the total atmospheric pressure.

p_{Fs} : is the pressure of saturation.

$$P_{Fs} = P_{amb} \exp\left[\frac{L_V M}{R}\left(\frac{1}{T_{eb}} + \frac{1}{T_S}\right)\right] \qquad (19)$$

The thermodynamic properties and transport properties are calculated at reference temperature and composition defined by the one - third rule '1 / 3 'suggested by Sparrow and Gregg (1958).

$$T_r = T_S + \frac{T_\infty - T_S}{3} \qquad (20)$$

$$Y_{Fr} = Y_{Fs} + \frac{Y_{F\infty} - Y_{FS}}{3} \qquad (21)$$

the latent heat of vaporisation is determined from the Watson relation

$$L_V = L_{VTeb}\left(\frac{T_{cr} - T_S}{T_{cr} - T_{eb}}\right)^{0.38} \qquad (22)$$

One assumption of the quasi-steady theory is to neglect the effects of natural convection. To quantify these effects on the vaporisation, a correction based on the Grashof and Prandtl numbers is introduced as

$$K_{corr} = K_{th}\left(1 + 0.5 Gr^{1/4} Pr^{1/3}\right) \qquad (23)$$

$$Gr = \frac{g\,\beta\,D^3\,\Delta T}{\upsilon^2} \qquad (24)$$

Where

g : is the gravity

β : is the gas compressibility coefficient

υ : is the cinematic viscosity.

$$Pr = \frac{\upsilon}{\lambda} \qquad (25)$$

3. Results and discussion

The following table presents the calculated surface temperatures and evaporation rates of each fuel. We observe that the surface temperature is greater for the fuel that has a high molecular weight, namely n-decane, so the difference between environmental temperature and the droplet surface is lower held out for the case of n-heptane, the difference between surface temperature and the middle is great. This temperature difference creates a temperature gradient that causes heat transfer to the droplet and consequently promotes evaporation.

	heptane	octane	nonane	decane
T_S (K)	274.6	285.5	292.5	296
$B_M = B_T$	0.0545	0.0277	0.012	0.004
K_{th}	0.0162	0.00651	0.00232	0.00071
K_{exp} (Birouk)	0.0150	0.00632	0.002013	0.00065

Figures 2, 3, 4 and 5 shows the variation of the diameter squared, normalized by the square of the diameter of the initial droplet, according to the discharge time was also normalized by the square of the diameter of the initial droplet for the four fuels for an environmental temperature of 373 K, these results are compared with experimental results obtained by C.Morin and I.Gokalp, 1999. The curves obtained were almost similar trends with the experimental. The four curves in these figures show that this variation is a linearly decreasing function of time. We also observed that reducing the diameter of the droplet is faster for the case of fuel which has the lowest molecular weight, namely n-heptane. The difference between the rates of fuel vaporisation is explained mainly by the difference of values of molar mass.

Figures 6, 7, 8 and 9 show the variation of the diameter squared, normalized by the square of the diameter of the initial droplet for the four fuels at different temperatures 373 to 673 K. we observe in these figures a net increase in the rate of evaporation as a function of temperature. However, each fuel responds differently to the same temperature and relative increase in the rate of evaporation with temperature is important for the more volatile fuel, namely n-heptane.

Figures 10, 11, 12 and 13 shows the theoretical results of the average vaporisation rate versus temperature for each fuel, these results are compared with experimental results obtained by C.Morin and I.Gokalp, 1999.
The curves obtained were almost similar trends with experimental, we also observed in these figures that the curve of the evaporation rate is important for the lighter fuel in case the n-heptane.
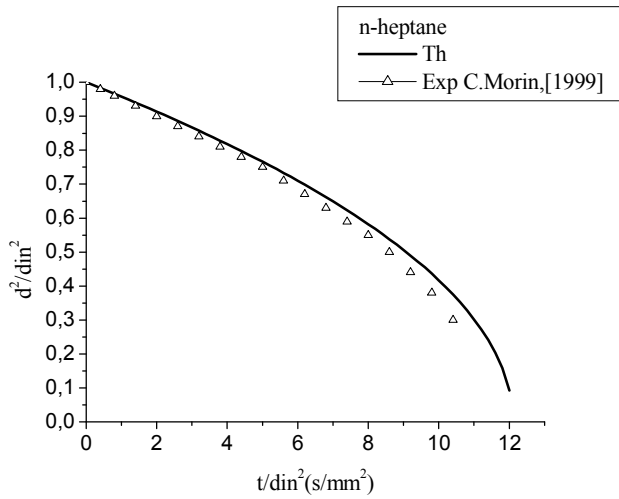
Fig.2. Temporal variation of droplet area with
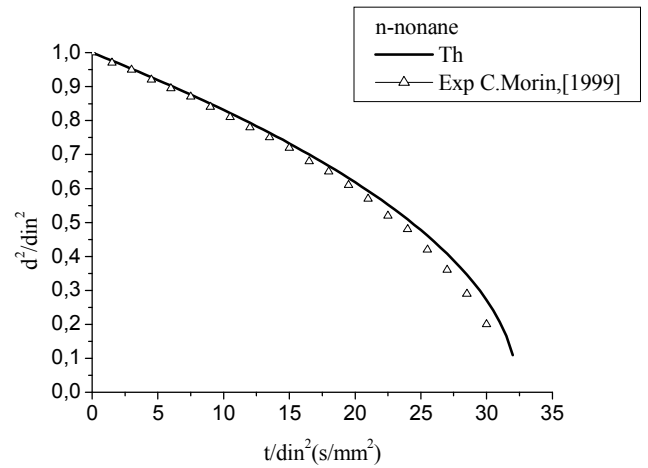initial diameter of n-heptane at T=373K

Fig.4. Temporal variation of droplet area with
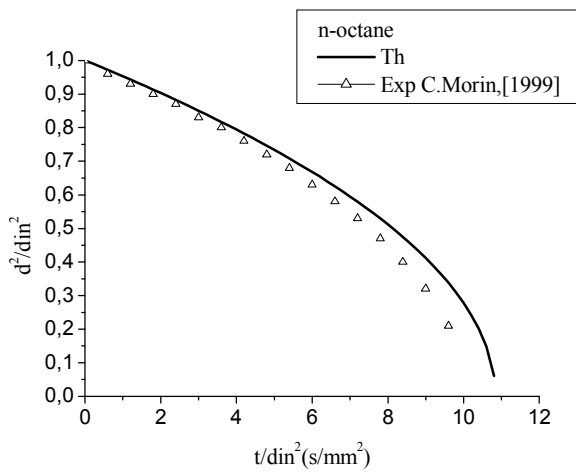initial diameter of n-nonane at T=373 K

Fig.3. Temporal variation of droplet area with
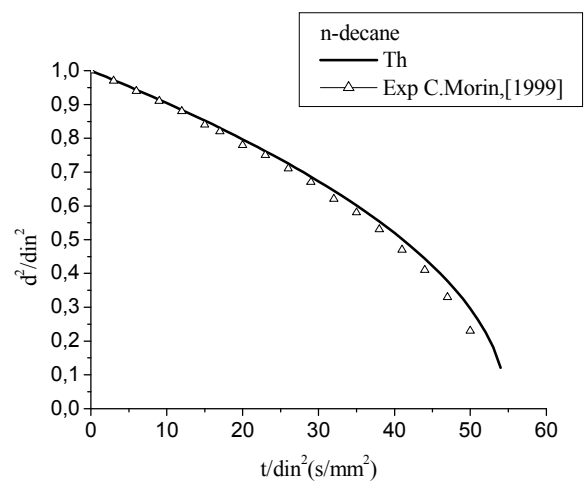initial diameter of n-octane at T=373 K

Fig.5. Temporal variation of droplet area with
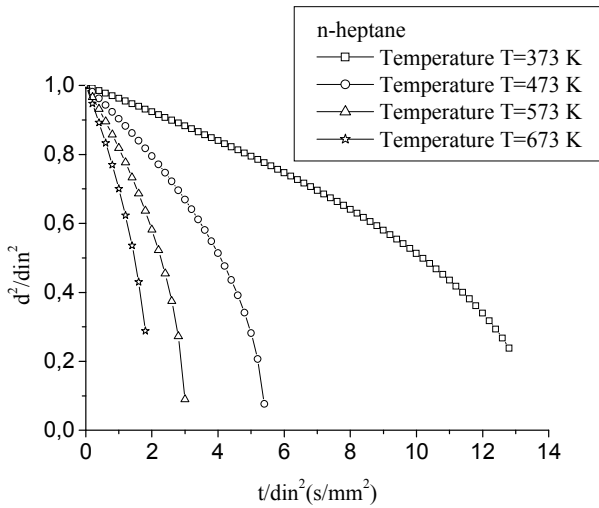initial diameter of n-décane at T=373 K

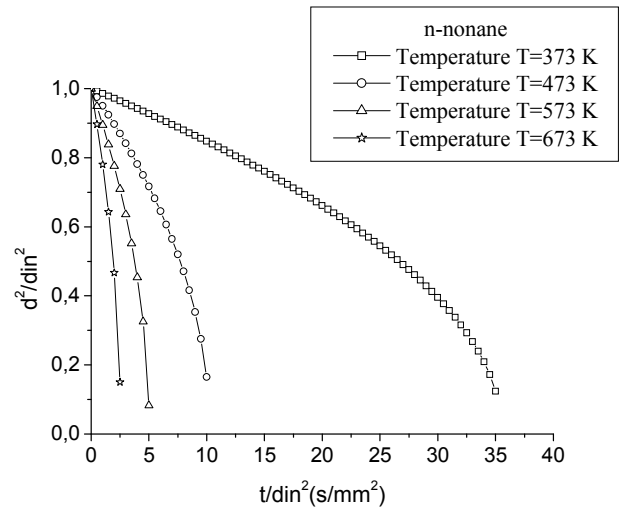Fig.6. Temporal variation of droplet area with initial diameter of n-heptane at different temperature

Fig.8. Temporal variation of droplet area with initial diameter of n-nonane at different temperature
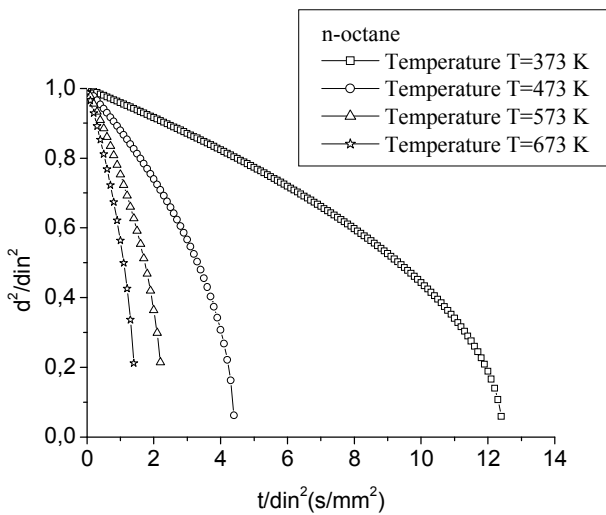

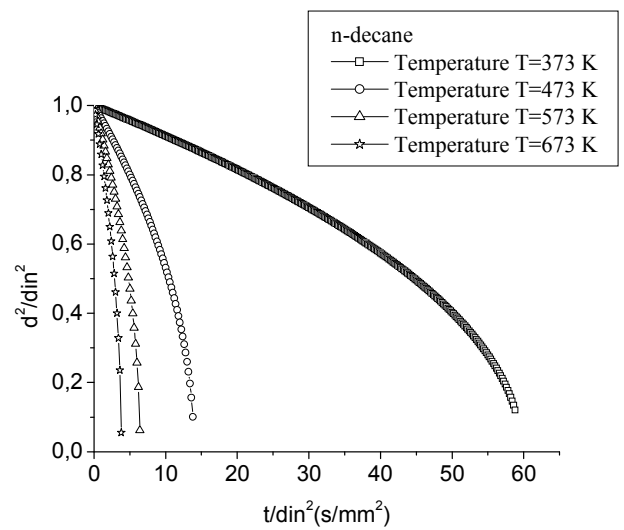Fig.7. Temporal variation of droplet area with initial diameter of n-octane at different temperature

Fig.9. Temporal variation of droplet area with initial diameter of n-decane at different temperature
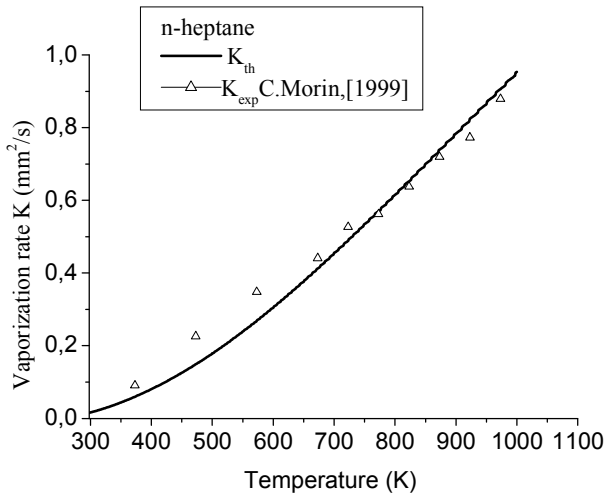
Fig.10. Evolution of average vaporisation rate
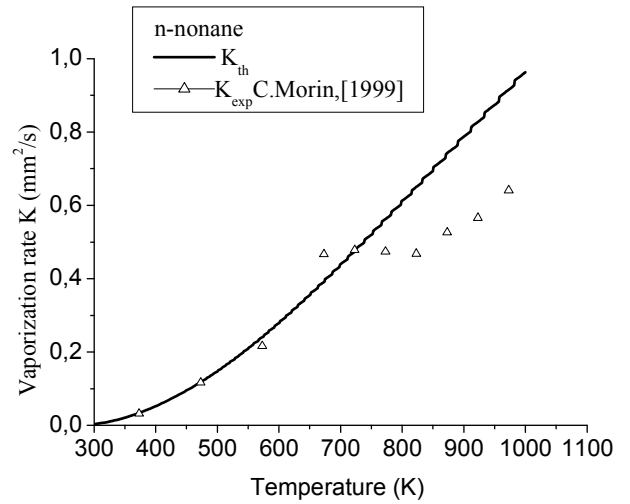for n-heptane versus temperature

Fig.12. Evolution of average vaporisation rate
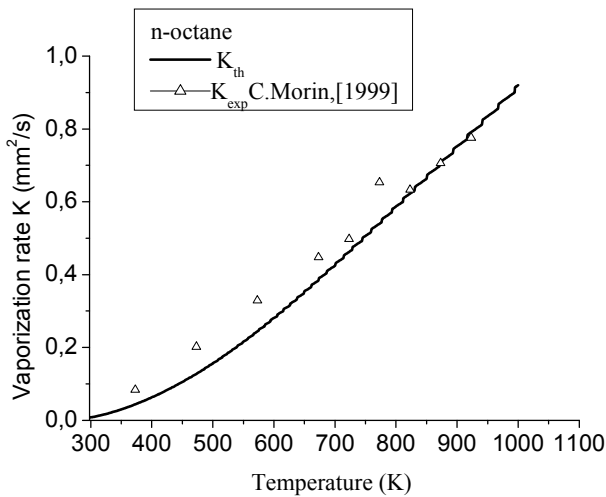for n-nonane versus temperature

Fig.11. Evolution of average vaporisation rate
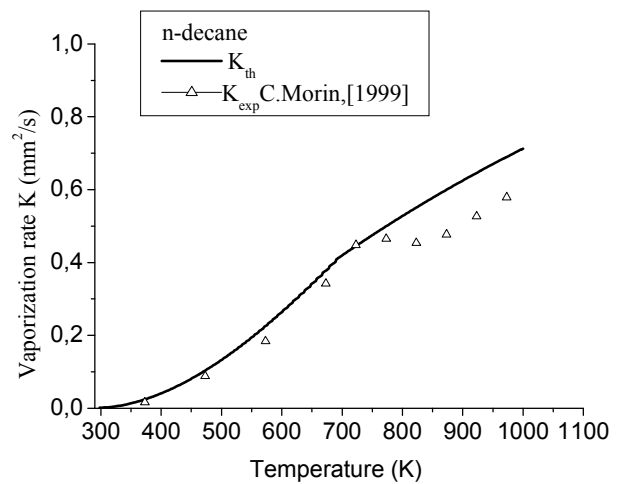for n-octane versus temperature

Fig.13. Evolution of average vaporisation rate
for n-decane versus temperature

Conclusion

The study we presented aims to identify and characterize the effect of temperature on the fuels droplets vaporisation. The results obtained by the quasi-steady theory are confronted with several test cases, including those obtained by M.Birouk, I.Gokalp, 1996 and C.Morin, I.Gokalp, 1999 under normal conditions pressure and temperature, then at different temperatures. was observed for the normal case the fuel that has a molar mass lower vaporizes rapidly, while the fuel has a higher molecular weight has a surface temperature lower and therefore the rate of evaporation very low. In if stagnant, with variation of temperature, the vaporisation rate is proportional to it, the more the temperature rises more fuel becomes more volatile.

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