Diffusion Coefficients of UAE Gasoline as Inputs to Some Environmental Transport or Risk Assessment

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Abstract—**Vapor diffusion was studied from volatile liquids of three brands of UAE gasoline: Super, Special, E+ and a mixture of these brands. The studying was conducted at 50 ^{o}C which represent the highest atmospheric temperature in UAE. The diffusion coefficients of Super gasoline (98 Octane number) was equal to 6.348 E-07, for special gasoline (95 octane number) equal to 7.353 E-07, for E+ (octane number 91) equal to 2.169 E-06, and the mixture of these three brands is 6.302E-07 m^2/s. This concluded that super gasoline which has the higher octane number, minimum density, and higher heat of combustion has the lowest diffusion coefficient with air.**

Index Terms—**Diffusion coefficient, gasoline with different octane number, risk assessment.**

I. THEORETICAL BACKGROUND

Molecular diffusion is defined as the random motions of molecules through different fluids which finally forming homogenous mixture. Usually the diffusion occurs from high concentration regions to low concentration regions. There are different factors that affect diffusion such as temperature, pressure and molecular weight. The diffusion occurs faster in high temperature, low pressure, and low molar mass.

The diffusivity of the vapor of a volatile liquid in air can be conveniently determined by Winklemann's method in which liquid is contained in a narrow diameter vertical tube, maintained at a constant temperature, and an air steam is passed over the top of the tube to ensure that the partial pressure of the vapor is transferred from the surface of the liquid to the air stream by molecular diffusion. The rate of mass transfer is given by [1] and [2]:

$$N_A = D\left(\frac{C_A}{L}\right)\left(\frac{C_T}{C_{BM}}\right)$$

Considering the evaporation of the liquid:

$$N_A = \left(\frac{\rho_L}{M}\right)\frac{dL}{dt}$$

Thus

$$\left(\frac{\rho_L}{M}\right)\frac{dL}{dt} = D\left(\frac{C_A}{L}\right)\left(\frac{C_T}{C_{BM}}\right)$$

Integrating and putting $L=L_o$ at $t=0$

$$L^2 - L_o^2 = \left(\frac{2MD}{\rho_L}\right)\left(\frac{C_A C_T}{C_{BM}}\right)t$$

$L-L_o$ can be measured accurately using the vernier on the microscope.

$(L-L_o)$ at time t = Initial reading on vernier – reading on vernier of time t.

$$(L-L_o)\ (L-L_o+2L_o) = \left(\frac{2MD}{\rho_L}\right)\left(\frac{C_A C_T}{C_{BM}}\right)t$$

Rearranging to solve for $\frac{t}{L-L_o}$

$$\frac{t}{L-L_o} = \left(\frac{\rho_L}{2MD}\right)\left(\frac{C_{BM}}{C_A C_T}\right)(L-L_o) + \left(\frac{\rho_L c_{BM}}{MD\ C_A C_T}\right)L_o$$

If m is the slope of the graph of $\frac{t}{L-L_o}$ versus $(L-L_o)$, then:

$$m = D = \left(\frac{\rho_L C_{BM}}{2mMC_A C_T}\right)$$

Diffusion coefficients, along with other parameters, are required inputs to some environmental transport or risk assessment models [3]. Literature values are sometimes available for these parameters, although, often the literature values are determined at 25 ^{o}C. Regulatory programs may have developed preferred sets of parameter values, which should be used if available. Further information on parameter sets is available on the chemical properties page. When parameter values are otherwise unavailable, either for an unusual chemical, or for a temperature not reported in the literature, a calculated value may be useful. Diffusion coefficients of different brands of gasoline are not available in any literature at any temperature.

Gasoline is refined from crude oil. It is a mixture of many different hydrocarbons. The gasoline is considered volatile or has high tendency to vaporize, and this is required to allow easy starting and drivability when the engine is cold. This is required in this particular experiment because it should vaporize and diffuse into the flowing air. However, extreme volatility results in failing of combustion because the liquid fuel has changed to a gaseous fuel in the fuel lines and this is known as "vapor-lock. In addition, it should not be so volatile because it might evaporate from fuel tank in the hot weather which affects the health and environment. Hence, the gasoline volatility is controlled by distillation and vapor pressure specification. In short,

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diffusion of gasoline in air is an important area of studying as it has an effect on both health and environment.

The most important difference between the three types of gasoline is in the octane rating. The higher the octane number is the slower the burn rate, and the greater the resistance to auto-ignition or knock of the fuel. The octane number of the three different types of the gasoline in this experiment super, special, and E+ are 98, 95, and 91, respectively. Hence, the best type is super. Moreover, these three types has different densities in which E+ is considered the lightest with the lowest density and super is the heavies with the highest density. E+ has the lowest lead content among the other two types. The diffusion of these three different types of gasoline as well as a mixture of the three types will be studied.

II. METHODOLOGY

A. Material

Three brands of gasoline were used with the properties shown in Table I.

TABLE I: GASOLINE SPECIFICATIONS

Property	ASTM method	E + (91)	Special (95)	Super (98)
Appearance	Visual	Clear and bright	Clear and bright	Clear and bright
Density at 15 ^oC.kg/l	ASTM D 1298	0.71-0.77	0.71-0.79	0.71-0.8
Distillation, oC	ASTM D 86			
10%		Max 65	Max 65	Max 70
50%		77-115	77 -115	77 -115
90%		Max 180	Max 180	Max 180
End point		max 205	Max 215	Max 215
Residue, vol.%		Max 2.0	Max. 2.0	Max. 2.0
Octane No. research	ASTM D 2699	Min 91	Min 95	Min 98
Octane No. motor	ASTM D 2700	Min 83	Min 85	Min 87
Reid vapor pressure@37.8 ^oC in summer, kg/cm^2	ASTM D 323	Max 0.6	Max 0.6	Max 0.6
Sulfur, ppm by wt	ASTM 1266	Max 100	Max 500	Max 500
Aromatic, vol%	ASTM D 1319	Max 40	Max 50	Max 55
Olefins , vol%	ASTM D 1319/5580	Max 10	Max 10	Max 10

B. Apparatus

The gas diffusion apparatus was used as shown in Fig. 1. The diffusion of a vapor ‘A’ from a volatile liquid into another gas ‘B’ can be conveniently studied by confining a small sample of the liquid in a narrow vertical tube, and observing its rate of evaporation into a stream of gas ‘B’ passed across the top of the tube. Normally, for simple instructional purposes, ‘B’ is air and ‘A’ is an organic solvent such as gasoline.

C. Experimental Work

Partially fill the capillary tube with gasoline and remove top nut from metal fitting. Connect flexible air tube to one end of the ‘T’ piece. With the microscope set up, adjust the object lens. Adjust the vertical height of the microscope until the capillary tube is visible. If it is not visible, adjust the distance from the object lens to the tank until it is. Switch on air pump (Airflow should only be low velocity across the capillary tube and can be adjusted using the Hoffman clip on the flexible tube). Record the level inside the capillary tube. Switch on temperature controlled water bath (adjust set point on controller to 50℃ and obtain a steady temperature.

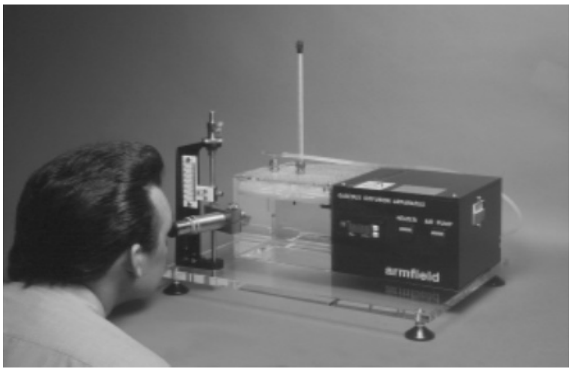

Fig. 1. Gaseous Diffusion coefficient apparatus

III. RESULT AND DISCUSSION

The graphs of $\frac{t}{L-L_o}$ versus (L-L_o) of these four trials were plotted as shown in Fig. 2-5.

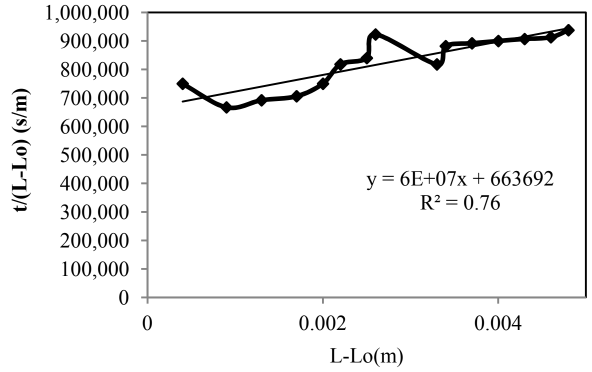

Fig. 2. Gasoline 95 Special Graph of (*t/L-Lo*) vs. (*L-Lo*)

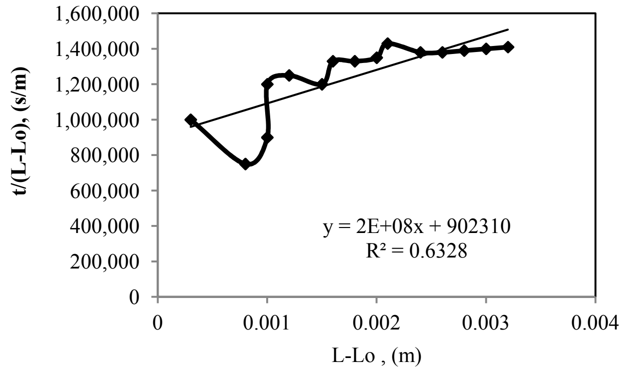

Fig. 3. Gasoline 91 E+ graph of (*t*/*L-Lo*) VS. (*L-Lo*)

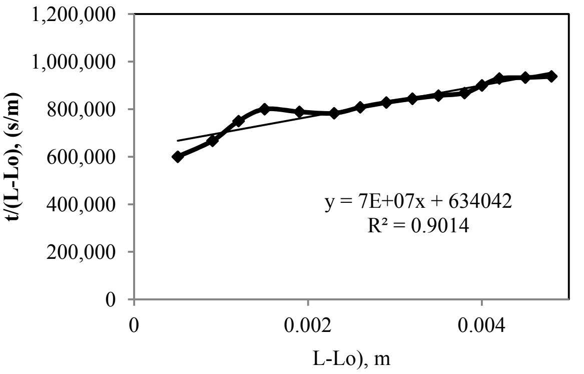

Fig. 4. Gasoline 98 graph of (*t/L-Lo*) vs. (*L-Lo*)

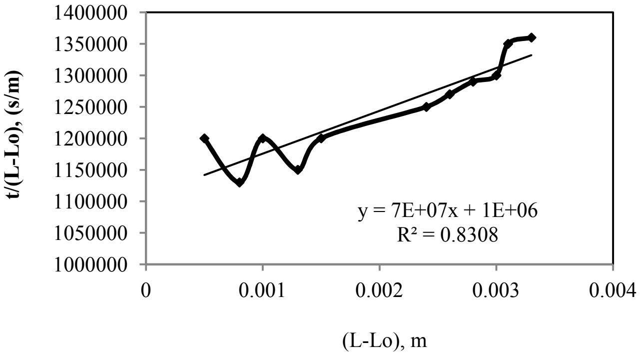

Fig. 5. Mixted brand gasoline graph of (*t/L-Lo*) vs. (*L-Lo*)

The diffusivity coefficient can be calculated by the use of Table II.

The diffusivity coefficient are shown ion Table III.

From this table, it is clear that gasoline E+ has the higher diffusion coefficient compared with others with lowest density and lowest octane number. It is clear that gasoline special (octane 98) has more resistance to diffuse into air. This gasoline has also highest heat of combustion so that the energy which can get is higher than the gasoline 95 and E plus gasoline. These results are in concise with theory that the lower density material has higher diffusion coefficient with air which means more environmental impact comparing with other types.

TABLE II: SPECIFICATION OF DIFFERENT BRANDS OF GASOLINE

	Gasoline 91 E+	Gasoline 95	Gasoline 98	Equi-mixture
Pa (atm)	1	1	1	1
CBM, (kMole/m^3)	0.0154	0.0154	0.01534	0.0154
ρL (kg/m3)	747.12	759.78	766.46	759.78
Pv-Gasoline (atm)	0.8869	0.8869	0.8869	0.8869
CB2 (kMole/m3)	0.00427	0.00427	0.00426	0.00427
CT (kMole/m3)	0.0377	0.0377	0.03769	0.0377
CA (kMole/m3)	0.0335	0.0335	0.03343	0.0335
MW	105	105	105	105
T , °C	50	50	50	50

TABLE III: DIFFUSIVITY COEFFICIENT OF DIFFERENT BRANDS OF GASOLINE

	Gasoline E+	Gasoline 95	Gasoline 98	Gasoline mixture
Diffusivity coefficient m^2/s	$2.169\text{x}10^{-6}$	$7.353\text{x}10^{-7}$	$6.348\text{x}10^{-7}$	$6.302\text{x}10^{-7}$

IV. CONCLUSION

Diffusion and other properties play an important rule to some environmental transport or risk assessment. It is important to include this value with other values especially with volatile liquids. Gasoline is one of these liquid which used for large quantities all over the world. It is found that this property relate with density and octane number of gasoline.

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NOMENCLATURE

C_A: Saturation conc. at interface [kmol/m^3]

C_{BM}: Logarithmic mean molecular conc. of vapor [kmol/m^3]

C_T: Total molar conc. = C_A+ C_{BM} [kmol/m^3]

D: Diffusivity or diffusion coefficient [m^2/s]

L: Effective distance of mass transfer [mm]

M: Gasoline Molecular Weight = 58.08 kg/mol

P_v: Gasoline vapor pressure (at 40°C) = 56kN/m^2

P_a: Atmospheric Pressure = 101.3 KPa

t= time (s)

T_{abs}: Absolute Temperature = 273

T_a : Temperature of gasoline in water bath.

ρ_L: Liquid Acetone density (at 40°C) = 790 kg/m^3

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