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Predicting the Liquid Lengths of Heavy Hydrogen Fuels

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Predicting the Liquid Lengths of Heavy Hydrogen Fuels

Laura L. Hoogterp

Abstract

The purpose of this paper is to outline the procedure used in determining the liquid lengths in diesel fuels. Using models formulated by previous researchers as well as the thermodynamic properties for three fuel surrogates the liquid length can be determined for diesel fuel, JP8 as well as provide a model for fuels between these ranges. This information is to later be used to develop a computer program to perform these calculations on engines running in a test cell.

Introduction

In order to predict the liquid length in diesel fuels three surrogate fuels are chose to model. Dodecane, C₁₂H₂₆, is used to model JP8, Hexadecane, C₁₆H₃₄, models diesel fuel, and Tetradecane, C₁₄H₃₀, is used to model fuel between these ranges.

Many people have previously done research into predicting the liquid lengths of diesel fuels. This information is then used to help predict liquid lengths for the three fuels. The models used are taken form the SAE technical paper by Dennis L. Siebers while the thermodynamic information on the fuels is found in books published by the American Petroleum Institute and a thermodynamics book.

These sources are used to find the liquid lengths which are then checked against existing data for hexadecane. Once the process is determined to be valid, the same procedure is followed for both tetradecane and dodecane. The method used is then broke down so that it can be used in a computer program that will predict the liquid lengths. The program will be used on engines that are running in a test cell. The rest of this paper will outline the procedure that is used to predict the liquid lengths in these fuels.

Modeling the Liquid Length

In order to determine the liquid length of fuels equations that have already been formulated through previous research are used. According to the SAE paper by Siebers the following equation is used to solve for the liquid lengths [1]:

$$L = \frac{b}{a} \sqrt{\frac{\rho_f}{\rho_a}} \frac{\sqrt{C_a} \cdot d}{\tan\left(\frac{\theta}{2}\right)} \sqrt{\left(\frac{2}{B(T_a, P_a, T_f)} + 1\right)^2 - 1}$$

where

L is the liquid length of the fuel,

b is a constant stated to be 0.41,

a is a constant found to be 0.66.

ρ_f is the density of the liquid fuel,

ρ_a is the density of the ambient gas,

C_a is the area contraction coefficient,

d is the diameter of the orifice,

θ is the spray spreading angle, and

$B(T_a, P_a, T_f)$ is the gas mass flow rate based on both enthalpies and compressibilities and solved for iteratively.

This value of B is solved for using the following equation [1]:

$$B = \frac{Z_a(T_s, P_a - P_s) \cdot P_s \cdot M_f}{Z_f(T_s, P_s) \cdot [P_a - P_s] \cdot M_a} = \frac{h_a(T_a, P_a) - h_a(T_s, P_a - P_s)}{h_f(T_s) - h_f(T_f, P_a)}$$

where

$Z_a(T_s, P_a - P_s)$ is the ambient air compressibility based on saturation temperature and partial pressure,

$Z_f(T_s, P_s)$ is the vaporized fuel compressibility based on the saturation temperature and pressure,

P_s is the saturation pressure of the fuel,

M_f is the molecular weight of the fuel,

$[P_a - P_s]$ is the partial pressure of the ambient gas, and

M_a is the molecular weight of the ambient gas.

On the enthalpy side of the equation,

$h_a(T_a, P_a)$ is the ambient gas enthalpy based on initial ambient temperature and pressure,

$h_a(T_s, P_a - P_s)$ is the ambient gas enthalpy based on saturation temperature and partial pressure,

$h_f(T_s)$ is the fuel enthalpy based on saturation temperature, and

$h_f(T_f, P_a)$ is the fuel enthalpy based on initial fuel temperature and pressure.

The compressibility of the ambient gas is assumed to be one. This assumption can be made when the pressure of the gas is low when compared to the critical pressure and/or the temperature is large relative to the critical temperature [3]. One or both of these conditions are met, which validates the assumption.

The compressibility of the fuel when it is a saturated vapor is found by interpolating numbers off a table found on the American petroleum institute's technical data book. To simplify this procedure so that it can be transformed into computer code a best fit curve of the data is found. A plot is created of the compressibility factor based on the reduced saturation temperature. A polynomial curve fit is then performed to obtain a relationship between temperature and compressibility for each fuel. These relationships should not be used outside the temperature range of 450 K to 1300 K to ensure the integrity of the curves.

For dodecane the relationship used to determine the compressibility is

$$Z_f = -16.85 \cdot T_{s,r}^3 + 36.104 \cdot T_{s,r}^2 - 26.425 \cdot T_{s,r} + 7.5406$$

where $T_{s,r}$ is the reduced saturation temperature of the fuel.

The tetradecane compressibility relationship is

$$Z_f = -17.924 \cdot T_{s,r}^3 + 36.143 \cdot T_{s,r}^2 - 24.71 \cdot T_{s,r} + 6.6857$$

and hexadecane's relationship is

$$Z_f = -16.587 \cdot T_{s,r}^3 + 34.594 \cdot T_{s,r}^2 - 24.531 \cdot T_{s,r} + 6.869$$

The enthalpy of the ambient gas is looked up in tables found in reference 3 and are based on either initial or saturation temperatures. To make calculations easier a relationship is formulated to determine these values. Since the enthalpies are taken over a wide range of temperatures they are broke up into smaller sections to keep the equation more accurate, and should not be used outside the stated temperature ranges. The enthalpy is in kJ/kg and the temperatures are in Kelvin.

For temperatures ranging for 450 K to 600 K the enthalpy is found using

$$h_a = 1.033 \cdot T - 13.605$$

For temperatures ranging from 600 K to 800 K

$$h_a = 1.0735 \cdot T - 37.788$$

temperatures between 800 K and 1000 K use

$$h_a = 1.1184 \cdot T - 73.254$$

and from 1000 K to 1320 K use the relationship

$$h_a = 1.1682 \cdot T - 123.49$$

To determine the enthalpy of the fuel in a gaseous state, a procedure is used out of the American Petroleum Institute data books. Two double integrations are performed and then the results plugged into an equation. Due to the complexity of this procedure the results are also plotted with a best fit curve for fuel in a gas and liquid state. For fuels at a reduced pressure less than 0.2 and in a gas state the following equations can be used [2]:

dodecane:
$$h_{f,v} = 1562.5 \cdot T_{r,s} - 444.84$$

tetradecane:
$$h_{f,v} = 1683.8 \cdot T_{r,s} - 469.88$$

hexadecane:
$$h_{f,v} = 1869.7 \cdot T_{r,s} - 550.15$$

where $h_{f,v}$ is the enthalpy of the fuel when it is a vapor.

If the reduced pressure of the vapor is greater than 0.2 then the following equations listed below are used. For the set of conditions given this occurs at 550 K in dodecane, 580 K in tetradecane, and 620 K in hexadecane. The equations are:

dodecane:
$$h_{f,v} = -1921.9 \cdot T_{r,s}^2 + 4996.7 \cdot T_{r,s} - 1978$$

tetradecane:
$$h_{f,v} = -3712.2 \cdot T_{r,s}^2 + 8085.6 \cdot T_{r,s} - 3229.2$$

hexadecane:
$$h_{f,v} = -929.51 \cdot T_{r,s}^2 + 3520.3 \cdot T_{r,s} - 1283.4$$

where h is given in kJ/kg.

To determine the enthalpy of the fuel in a liquid state the following equations are used. They are based on pressure rather than temperature since the fuel entering the system is at a constant temperature. Enthalpy is in kJ/kg.

$$\text{dodecane: } h_{f,l} = 1.277 \cdot P_{a,r} + 316.3$$

$$\text{tetradecane: } h_{f,l} = 1.1718 \cdot P_{a,r} + 319.12$$

$$\text{hexadecane: } h_{f,l} = 1.0429 \cdot P_{a,r} + 320.95$$

where,

$P_{a,r}$ is the reduced ambient pressure with respect to the fuel and

$h_{f,l}$ is the enthalpy of the fuel in a liquid state.

To calculate the spray spreading angle the following equation is used [1]:

$$\tan\left(\frac{\theta}{2}\right) = c \cdot \left[\left(\frac{\rho_a}{\rho_f} \right)^{0.19} - .0043 \cdot \sqrt{\frac{\rho_f}{\rho_a}} \right]$$

where

c is a constant based on the orifice diameter and is 0.26 for a diameter of 246 μm .

To determine the fuel density in its liquid state the following equation is used [2]:

$$\frac{1}{\rho_s} = \left(\frac{RT_c}{P_c} \right) Z_{ra}^{[1+(1-T_r)^{2/7}]}$$

where

ρ_s is the saturated liquid density,

P_c is the critical pressure of the fuel,

$T_{f,r}$ is the fuel temperature reduced, and

Z_{ra} is an empirically derived constant that can be found in reference 2.

Since the equation came from reference 2 and the formulation of the constants is unknown, the critical pressure must be inputted in psi. This produces density with units of $\frac{\text{lb} - \text{mol}}{\text{ft}^3}$ and can then be converted to SI units.

The ambient and saturation pressure are used in determining many properties. In order to find the ambient pressure before fuel enters the system the ideal gas law is used [3]:

$$P_a = \rho_a RT_a$$

where

R is the ideal gas constant,

P_a is the ambient pressure, and

T_a is the ambient temperature.

To find the vapor pressure of the fuel based on its temperature the correlation

$$\ln P_s = A + \frac{B}{T_s} + C \ln T_s + D T_s^2 + \frac{E}{T_s^2} \text{ is used [2].}$$

A, B, C, D, and E are constants based on the fuel in question. It should be noted that the T should be in degrees Rankine and the equation produces a pressure in psi.

Results

A spreadsheet in excel is set up in order to perform the calculations necessary to determine the liquid length of the three fuels. In order to check the results from excel with the work previously done by Siebers the same set of conditions are used. The ambient gas densities used are 3.6, 7.3, 14.8, 30.2, 59.0 kg/m³.

In Seiber's research the ambient gas conditions have a composition of 89.7% N₂, 6.5% CO₂, and 3.8% H₂O with a molecular weight of 28.67 [1]. The excel sheet uses air as its ambient gas and the appropriate thermodynamic properties. This difference can cause a difference of 4% in the final liquid length due to heat capacities [1].

The injected fuel temperature is assumed to be 438 K, and the orifice diameter is 246 μm. The liquid length is then measured at 700 K, 850 K, 1000 K, 1150 K, and 1300 K. Using a table in Siebers report the area contraction coefficient is assumed to be 0.8124.

These conditions coupled with the equations listed above are used to iteratively solve for B. The conditions are determined at a variety of saturation temperatures at the each of the ambient temperatures and densities. The equation for B is then solved to within a hundredth of each other. It is at this point that the liquid length can be determined. Table 1 is a sample of the excel sheet created.

Table 1: Excel sheet created to find the liquid length of hexadecane with ambient conditions at 850 K and a density of 30.2 kg/m³

Knowns:										Pressure	
a	b	ρ_{air} [kg/m ³]	Ca	Mair	Mfuel	d	tan $\theta/2$			Pa [Pa]	Pa [Mpa]
0.65	0.41	30.2	0.8124	28.97	226.45	0.00025	0.139337			7366944	7.366944
Tf [K]	Ta [K]	ρ_{fuel} [kg/m ³]	Tc,air [K]	Tc,fuel [K]	Pc,air [Mpa]	Pc,fuel [Mpa]	Tr,fuel	Pr,ambient	acentric factor		
438	850	662.939	133	723	3.77	1.40006	0.607864	5.2618848	0.7174		

Iterations															
for Ts [K]	Tr,fuel [K]	Ps [MPa]	Pr,fluid [MPa]	Pa-Ps [MPa]	Za(Ts,Pa-Ps) []	Zf(Ts,Ps) []	ha(Ta,Pa) [kJ/kg]	ha(Ts,Pa-Ps) [kJ/kg]	hf(Tf,Pa) [kJ/kg]	hf(Ts) [kJ/kg]	B(z) []	B(h) []	difference []	Average B []	Liquid length [m]
450	0.622	0.00427	0.0031	7.363	1	0.97297	877.175	451.8	325.74	626.4521	0.004664	1.4	-1.4099	0.709612	0.01706802
500	0.692	0.02256	0.0161	7.344	1	0.95738	877.175	503.02	325.74	744.8596	0.025077	0.9	-0.86764	0.458897	0.02438106
550	0.761	0.08132	0.0581	7.286	1	0.92846	877.175	554.74	325.74	870.8941	0.093975	0.6	-0.49748	0.342716	0.03131938
600	0.83	0.22607	0.1615	7.141	1	0.85258	877.175	607.02	325.74	1002.705	0.290263	0.4	-0.1088	0.344665	0.03116484
650	0.899	0.52573	0.3755	6.841	1	0.72489	877.175	659.84	325.74	1123.17	0.82867	0.3	0.556126	0.550607	0.02094906
700	0.968	1.08217	0.7729	6.285	1	0.48614	877.175	713.27	325.74	1251.834	2.768636	0.2	2.591651	1.472811	0.00989018
610	0.844	0.27092	0.1935	7.096	1	0.83331	877.175	617.53	325.74	1028.355	0.358136	0.4	-0.0114	0.363839	0.02973227
620	0.858	0.32255	0.2304	7.044	1	0.81172	877.175	628.07	325.74	1053.211	0.440925	0.3	0.098499	0.391676	0.02789959
630	0.871	0.38168	0.2726	6.985	1	0.78668	877.175	638.63	325.74	1078.656	0.542928	0.3	0.215018	0.435419	0.02548809
640	0.885	0.44912	0.3208	6.918	1	0.7576	877.175	649.22	325.74	1104.807	0.66985	0.3	0.367087	0.486306	0.023222

The saturation temperature occurs at 610 K. This is determined because at this point the difference between the two values for B is only 0.0114. The liquid length value is read at this point and is 29.73 mm for hexadecane at an ambient temperature of 850 K and ambient gas with a density of 30.2 kg/m³.

While performing these calculations the difference in the B values drives the accuracy of the liquid length. When these values differ by hundredths the liquid length is only accurate to 1 mm. For this reason the computer program should be wrote so that the B values are within at least thousandths of each other to ensure the most accurate liquid lengths.

This process is repeated for each of the five ambient temperatures and the five ambient densities for the three fuels. In order to check this process hexadecane is done first. The data collected from the excel sheet is then compared to the values that are read off a chart in the SAE paper wrote by Siebers. Table 2 compares the liquid lengths for hexadecane:

Table 2: Liquid length values compared to previous research done for hexadecane at the stated conditions

Ambient Temperature [K]	Liquid Lengths [mm]									
	Density [kg/m ³]		7.3		14.8		30.2		59	
	Seiber's Research	Calculated Results	Seiber's Research	Calculated Results	Seiber's Research	Calculated Results	Seiber's Research	Calculated Results	Seiber's Research	Calculated Results
700	-	-	86	89.89	63	66.31	48	47.16	37	37.01
850	88	90.47	60	61.49	41	42.07	29	29.72	21	20.73
1000	72	71.43	47	48.14	32	31.71	21	21.38	15	15.67
1150	61	62.79	40	39.48	28	25.88	17	17.21	12	12.35
1300	55	54.46	35	35.40	23	23.08	14	15.18	10	9.76

It can be seen from this table that the values compare relatively well. Any discrepancies can be explained by the difference in ambient conditions as well as the fact that Seiber's values for the liquid length were estimated by reading them off a chart.

The results for the three fuels are summarized in the following tables and figures. It is seen that all the fuels follow the same basic trends and are all reasonable.

Dodecane:

Table 3: Liquid length values for dodecane at the stated conditions

Temperature [K]	Liquid Length [mm]				
	Density [kg/m ³]				
	3.6	7.3	14.8	30.2	59
700	86.83	61.26	42.58	30.76	23.67
850	65.95	43.24	30.72	21.02	15.64
1000	54.78	36.19	24.69	16.66	11.33
1150	47.57	31.22	20.55	13.66	9.65
1300	43.20	27.40	17.97	12.17	8.01

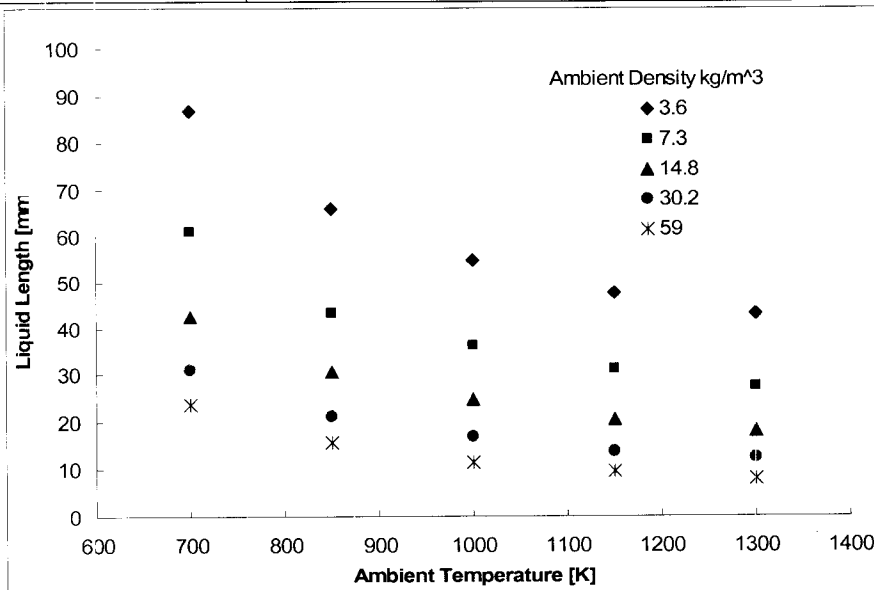


Figure 1: The liquid length of dodecane at varying ambient temperatures and densities

Tetradecane:

Table 4: Liquid length values for tetradecane at the stated conditions

Temperature [K]	Liquid Length [mm]				
	Density [kg/m ³]				
	3.6	7.3	14.8	30.2	59
700	106.62	76.69	54.19	39.65	29.92
850	83.38	54.61	37.23	25.75	18.49
1000	67.97	43.75	29.22	19.60	13.58
1150	58.61	37.50	24.32	16.21	10.77
1300	51.53	32.91	20.94	13.80	8.84

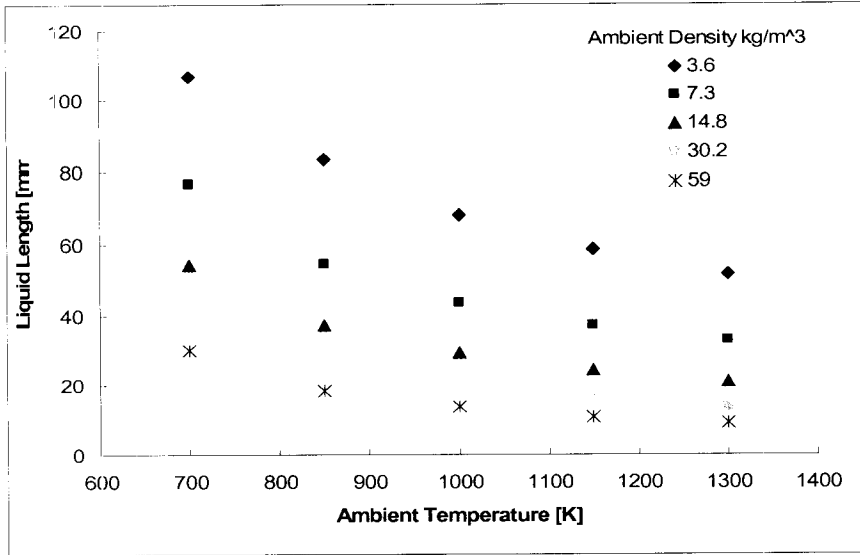


Figure 2: The liquid length of tetradecane at varying ambient temperatures and densities
Hexadecane:

Table 5: Liquid length values for hexadecane at the stated conditions

Temperature [K]	Liquid Length [mm]				
	Density [kg/m ³]				
	3.6	7.3	14.8	30.2	59
700	-	89.89	66.31	47.16	37.01
850	90.47	61.49	42.07	29.72	20.73
1000	71.43	48.14	31.71	21.38	15.67
1150	62.79	39.48	25.88	17.21	12.35
1300	54.46	35.40	23.08	15.18	9.76

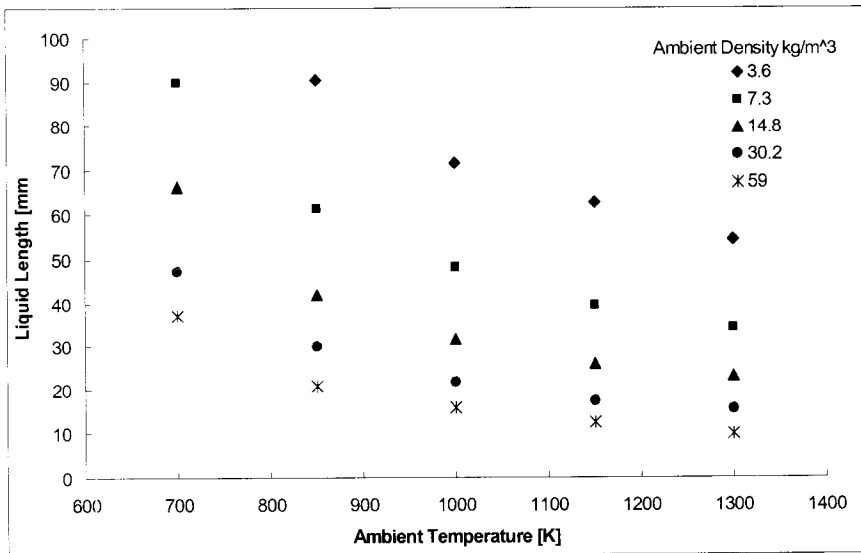


Figure 3: The liquid length of hexadecane at varying ambient temperatures and densities

Conclusion

It is determined that this method of determining the liquid length in the three diesel fuel surrogates is accurate. By using the equations previously found as well as thermodynamic properties the liquid lengths can successfully be determined. This is confirmed by comparing the data with the results previously obtained by Siebers.

Once the process is confirmed the procedure is repeated for the two remaining fuels. Some methods for finding the properties of the fuel in the combustion chamber are then simplified using best fit curves. These simplifications were then tested by running the calculations using the new equations and comparing them to the original data. It was found that the differences in the liquid lengths caused by these simplifications are negligible.

In the end it is determined that the procedures outlined in this paper are suitable for use in the creation of a computer program. The program should successfully be able to predict the liquid length in diesel fuels.

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