



Determining the Thermodynamic Properties of Fuel Blends from those of their Components For Air-Fuel Models of IC Engines

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Abstract: The paper presents an Excel-based procedure for determining the coefficients in the polynomials that describe the thermodynamic properties of fuel blends. The procedure is meant for use in conjunction with air-fuel computer models of internal combustion engines. It enables such models to deal with fuel blends just as they deal with pure fuels without modifying the main computer program. To obtain the mixture properties, the procedure applies the ideal-gas mixture relationship, which is already inherent in the formulation of existing air-fuels models. Excel has been chosen as computational platform for developing the procedure because of its simplicity and wide availability. The procedure is applied to determine the coefficients for binary mixtures of gasoline-ethanol, gasoline-hydrogen, and methane-hydrogen.

Keywords: Air-fuel models; Fuel-induction engines; Fuel blends; Thermodynamic properties.

1. INTRODUCTION

Theoretical models of internal combustion engines are design tools can be used to explore the effects of various operating parameters on the engine's performance. Compared to experimental methods, theoretical models have the advantage of being more flexible and less costly. The models can be grouped into three types of increasing of complexity: (a) closed-system air-standard models (b) closed-system air-fuel models, and (c) open-system air-fuel models. The first level includes the Otto and Diesel cycles as described in standard thermodynamics textbooks [1]. The practical limitations of these models, together with the availability of powerful personal computers and software, motivated researchers and engine designers to develop more realistic models. By adopting a fuel-air approximation rather the standard-air approximation, these models take into account the type of fuel used and the products of the combustion process, the composition of the exhaust gas, etc. [2,3]. The models also take into consideration the heat losses. While the second level of I.C. engine models also treat the engine cylinder as a closed system [2], the models of the third-level go a step further by treating the cylinder as an open system to take into account the mass losses [3]. Ferguson [3] described theoretical air-fuel models for both fuel-induced and fuel-injected engines treat the engine as an open system. The models allow for the effects of suction and discharge of the fluids involved and take account of the heat-transfer and mass transfer losses that take place. A

system of first-order ordinary differential equations is obtained for the pressure, volume, temperature of the burned and unburned gases, heat transfer, mass flow into and out of crevices, and the composition of combustion products. The equations can be solved on a personal computer using standard numerical techniques and computer software. Apart from detailing the theoretical formulation, Ferguson [3] also provided computer codes for these models in FORTRAN. His model has been adopted by other researchers using different programming platforms [4,5]. For example, Chai [4] wrote his model in Visual Basic while Buttsworth [5] used Matlab.

For practical considerations, the alternative fuels for I.C. engines are more commonly used as mixtures with conventional fossil fuels than in their neat form [6-8]. However, most previous studies that used theoretical models considered only pure fuels [9-14]. Existing air-fuel models determine the thermodynamic properties of the fuels from a set of polynomials. The models can be used to analyse the performance of internal combustion engines with fuel mixtures provided that the values of the coefficients in these polynomials can be determined. The present paper presents a procedure to determine the values of the coefficients for fuel mixtures from those of the pure components. The paper describes the mathematical and computational formulations of the procedure. Excel has been chosen as computational platform for developing the procedure because of its simplicity and wide availability. Apart from minimizing the programming effort, the Excel

sheet does not need a compiler and automatically updates its calculations once the data of the blend's components or their concentrations are changed. The Excel-based procedure is used to determine the relevant values for gasoline-ethanol, gasoline-hydrogen, and methane-hydrogen blends.

2. Thermodynamic Properties of Air, Fuels and Combustion Products

To evaluate the thermodynamic properties of the air and combustion products, the computer-based air-fuel models use a set of temperature-dependent polynomials. The following expressions were proposed by McBride et al [15] for air components and combustion products:

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (1a)$$

$$\frac{h}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + a_6 \frac{1}{T} \quad (1b)$$

$$\frac{s}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \quad (1c)$$

where R is the gas constant, T is the temperature in K , cp is the specific heat at constant pressure, h is the specific enthalpy and s is the specific entropy. McBride et al [15] calculated the coefficients a_1 to a_7 over two different temperature ranges: $300 < T < 1000$ K; and $1000 < T < 5000$ K. For the species of interest during combustion (CO_2 , H_2O , N_2 , O_2 , CO , H_2 , H , O , OH and NO) the values of the seven coefficients can be found in [3-5,17].

Slightly different forms of the polynomials were used to evaluate the thermodynamic properties of fuels (in vapour phase) [3-5,17]:

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 \frac{1}{T^2} \quad (2a)$$

$$\frac{h}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 - \frac{a_5}{T^2} + a_6 \frac{1}{T} \quad (2b)$$

$$\frac{s}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 - \frac{a_5}{2} \frac{1}{T^2} + a_7 \quad (2c)$$

Heywood [17] and Ferguson [3] adopted simplified versions of Eqs. (2) in which both a_4 and a_5 were set to zero. Buttsworth [4] checked the accuracy of this simplification.

Unlike the original FORTRAN codes provided by Ferguson [3], the air fuel models developed by Buttsworth [4] and by Chai [5] kept the fuel data in separate subroutines rather than being in the main body of the computer program. This makes the selection of the fuel more convenient to the user. It is also possible to add a new fuel by extending the fuel-data subroutine without any modifications to the main program. Thus, these air-fuel models can also be used to analyse the performance of IC engines with fuel mixtures by adding the mixture as a new fuel for which the values of the seven coefficients need to be determined.

3. Determining the Thermodynamic Properties of Fuel Blends

For fuel blends, values of the different coefficients in the polynomials of Equation (2) can be determined by making use of the fact that air-fuel models treat fuel vapours as ideal gases. Therefore, properties of the fuel mixture can be obtained from those of the various species from [18]:

$$\xi_{mixture} = \sum_{k=1}^N x_k \cdot \xi_k \quad (3)$$

where ξ refers to the property and x to the mass fraction of the mixture component. Equation (3) is usually used to determine mixture properties like specific heats and enthalpies. However, it can also be used to calculate the values of coefficients in Equations (2) for a fuel mixture from the respective values of its pure fuel components if the properties of the pure components are described by the same polynomial [18]. The equation cannot be used if the polynomials have different forms. A good example of this situation is when hydrogen is used as fuel extender for gasoline or natural gas. In this case, hydrogen is described by the polynomials of Equation (1) while gasoline and natural gas are described by the polynomials of Equation (2). The procedure described here does not apply Equation (3) to the coefficients themselves, but to the thermodynamic properties h and s . Since h and s of the fuel components can be obtained from different polynomials (or even given as discrete values), the procedure is more general than Equation (3). Given the enthalpy of the mixture at six selected temperatures and the entropy at the seventh temperature, the procedure determines the seven coefficient in Equation (2). An algebraic system is formed involving the values of the selected temperatures (as known) and the values of the seven coefficients (as unknown) as follows:

$$\begin{bmatrix} 1 & T_1/2 & T_1^2/3 & T_1^3/4 & T_1^4/5 & 1/T_1 & 0 \\ 1 & T_2/2 & T_2^2/3 & T_2^3/4 & T_2^4/5 & 1/T_2 & 0 \\ 1 & T_3/2 & T_3^2/3 & T_3^3/4 & T_3^4/5 & 1/T_3 & 0 \\ 1 & T_4/2 & T_4^2/3 & T_4^3/4 & T_4^4/5 & 1/T_4 & 0 \\ 1 & T_5/2 & T_5^2/3 & T_5^3/4 & T_5^4/5 & 1/T_5 & 0 \\ 1 & T_6/2 & T_6^2/3 & T_6^3/4 & T_6^4/5 & 1/T_6 & 0 \\ \ln(T_7) & T_7 & T_7^2/2 & T_7^3/3 & T_7^4/4 & 0 & 1 \end{bmatrix} \begin{Bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \\ a_7 \end{Bmatrix} = \begin{Bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \\ h_6 \\ s_7 \end{Bmatrix} \quad (4)$$

The above system of algebraic equations can be put in matrix notation as follows:

$$[T_i] \{a_i\} = \{\xi_i\} \quad (5)$$

where, T_i stands for the selected temperatures and ξ_i stands for either h_i or s_i . Solving the algebraic system determines the seven coefficients for the mixture.

Considering the small size of the system, it can be solved by the matrix inversion method, i.e.:

$$\{a_i\} = [T_i]^{-1} \{\xi_i\} \quad (6)$$

The procedure can be broken up into the following five steps :

1. Select the volume fractions of the mixture components and provide the coefficients $a_1 - a_7$ for each component
2. Provide the enthalpies of the mixture at six selected temperatures and the entropy at the seventh temperature (e.g. from Equations 2 or 3) and store in the property vector $\{\xi_i\}$
3. Construct the coefficient matrix $[T_i]$ in Equation (5)
4. Invert the coefficient matrix and store as $[T_i]^{-1}$
5. Multiply the inverted system $[T_i]^{-1}$ by the property vector $\{\xi_i\}$ to obtain the coefficient vector $\{a_i\}$ from Equation (6).

The procedure which requires a numerical solution can easily be programmed in Microsoft Excel. Figure 1 shows the Excel sheet where the parts corresponding to the five steps of the procedure have been labelled by respective numbers. The fuel's percentages and their coefficients are

entered in part (-1) of the sheet. In part (-2), the values of the mixture properties (h and s) are provided (or calculated by Equation 3) at seven selected temperatures and stored as $hm_1 - sm_7$. The coefficient matrix is then constructed in part (-3) and Excel's MINVERSE function is used in part (-4) to invert it. In part (-5), the matrix-multiplication function of Excel (MMULT) is used to multiply the inverted matrix with the property vector ($hm_1 - sm_7$) to obtain the values of the coefficients ($a_1 - a_7$) for the specified mixture shown in cells D36-D42. To verify the procedure, it was used to calculate the coefficients for a gasoline-ethanol mixture with 10% ethanol. Table 1 compares the results with the values obtained directly from Equation (3) at values of the temperature in the range 300 – 1000K. Note the modifications made to the algebraic system so as force the values of the two coefficients a_4 and a_5 to be zeros. Due to round-off error, Excel does not give exact zeros for the coefficients, but small values of order 10^{-20} .

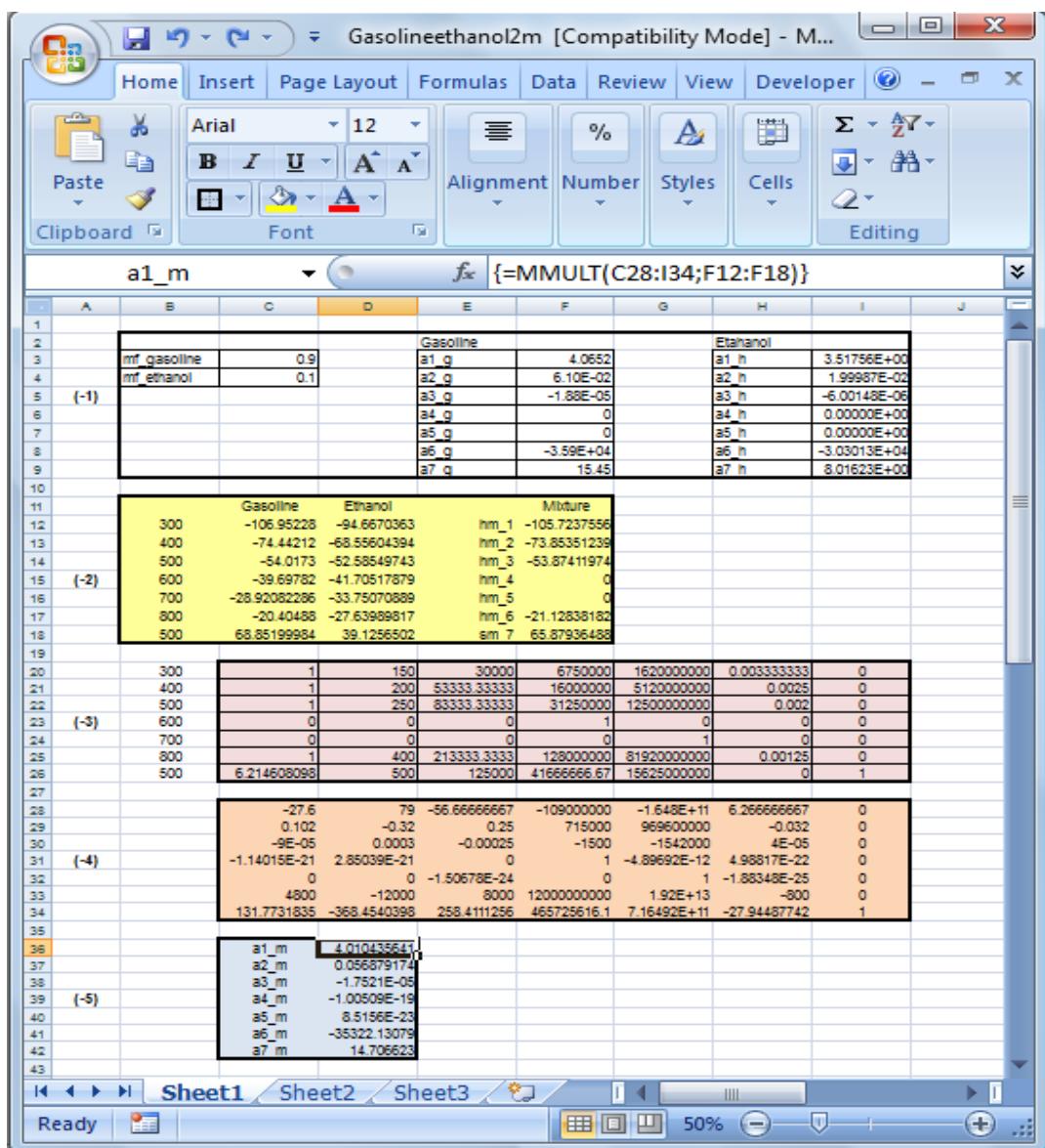


Figure (1). Excel sheet of the procedure.

4. Applications to Binary Mixtures

The Excel sheet shown on Figure 1 can be used to determine the coefficients for other gasoline-ethanol blends by only modifying the percentages of gasoline and ethanol stored in cells C3 and C4. Excel automatically updates all the following calculations and shows the new values of the coefficients in cells D36-D42. Table 2 gives the values of the coefficients for gasoline-ethanol blends with 5%, 10%, 15% and 20% ethanol concentrations. The values for the coefficients a_4 and a_5 , which are taken as zeros, are not shown on the table. The Excel sheet of Figure 1 can be used to calculate values of the coefficients for binary mixtures of other fuels by suitably modifying parts (-1) and (-2) of the sheet. Table 3 shows the calculated values of the coefficients for gasoline-hydrogen blends with different percentages of hydrogen while Table 4 shows the same for methane-hydrogen blends.

Table (1). Values of the coefficients for gasoline-ethanol mixture with 10% ethanol as obtained by Equations (3) and the present procedure

T (K)	Value by Eq. (3)	Value by Eq. (4)
a_1	4.010435641	4.010435641
a_2	0.056879174	0.056879174
a_3	-1.7521E-05	-1.7521E-05
a_4	-2.30393E-18	0
a_5	2.2367E-21	0
a_6	-35322.13079	-35322.13079
a_7	14.706623	14.706623

Table (2). Coefficients for a gasoline-ethanol mixture with different percentages of ethanol

Coefficients	5%	10%	15%	20%
a_1	4.037817821	4.010435641	3.983053462	3.955671283
a_2	0.058928087	0.056879174	0.054830261	0.052781348
a_3	-1.8161E-05	-1.7521E-05	-1.68811E-05	-1.62411E-05
a_6	-35601.06539	-35322.13079	-35043.19618	-34764.26157
a_7	15.0783115	14.706623	14.3349345	13.963246

Table (3). Coefficients for a gasoline-hydrogen mixture with different percentages of hydrogen

Coefficients	5%	10%	15%	20%
a_1	4.029968781	3.994737562	3.959506343	3.924275125
a_2	0.057952458	0.054927916	0.051903374	0.048878832
a_3	-1.78771E-05	-1.69532E-05	-1.60293E-05	-1.51054E-05
a_6	-34137.01808	-32394.03616	-30651.05423	-28908.07231
a_7	14.49887428	13.54774856	12.59662283	11.64549711

Table (4). Coefficients for a methane-hydrogen mixture with different percentages of hydrogen

Coefficients	5%	10%	15%	20%
a_1	2.040786581	2.110249162	2.179711743	2.249174325
a_2	0.007502315	0.007133043	0.006763772	0.0063945
a_3	-1.01231E-06	-9.76021E-07	-9.39736E-07	-9.0345E-07
a_6	-9484.918978	-9039.415955	-8593.912933	-8148.40991
a_7	8.251415878	7.629103757	7.006791635	6.384479513

5. Concluding Remarks

The Excel sheet developed for binary mixtures can be used to deal with tertiary mixtures by a straight-forward extension. This requires modifying only parts (-1) and (-2) of the sheet shown on Figure 1. Part (-1) should be modified to add the percentage of the third components and its seven coefficients. Part (-2), that calculates the mixture properties from Equation (3), should be modified to allow for the contribution of the third component in the mixture properties. No modifications are required for the three other parts of the sheet. It should also be noted that known discrete tabulated values of the mixture properties, or its components, can be entered in part (-2). The sheet will then proceed to calculate the mixture coefficients in the usual way.

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