

Enhancing Instruction in Fuels and Combustion Laboratory via a Developed Computer-assisted Program for Establishing Efficient Coal–Diesel Oil Mixture (CDOM) Fuel Proportions*

ARCHIE B. MAGLAYA

Department of Mechanical Engineering, De La Salle University, 2401 Taft Avenue, Malate Manila, Philippines. E-mail: maglayaa@dlsu.edu.ph

This paper discusses the relevance of digital computation in Fuels and Combustion Laboratory Experiments used by the senior students of the Department of Mechanical Engineering, De La Salle University-Manila, Philippines. One of the students' experiments involved the determination of the most efficient CDOM fuel proportion as alternative fuel to diesel oil for steam generators and other industrial applications. Theoretical calculations show that it requires tedious and repetitive computations. A computer-assisted program was developed to lessen the time-consuming activities. The formulation of algorithms were based on the system of equations of the heat interaction between the CDOM fuel, combustion air and products of combustion and by applying the principles of mass and energy equations (or the First Law of Thermodynamics) for reacting systems were utilized. The developed computer-assisted program output verified alternative fuel selected through actual experimentation.

INTRODUCTION

EDUCATION as a continuing learning process requires new trends and innovations to cope with the advance thinking of the students of modern generations. Engineering educators must be equipped with advanced techniques necessary to enhance instruction for an effective learning. It is in this sense that this paper discusses the relevance of digital computation used in one of the experiments performed by the senior students of the Department of Mechanical Engineering, De La Salle University-Manila, Philippines in their Fuels and Combustion Laboratory subject. This paper also presents one of the developed computer-assisted programs used in the students' experiments. The developed program is written in HyperText Markup Language (HTML[©]) and Javascript[©] for Microsoft Internet Explorer[©] 5.0 format. This will free the students from the tedious and laborious theoretical calculations in the determination of the adiabatic flame temperature as the basis for establishing an efficient CDOM fuel proportion as alternative fuel to diesel oil before an actual experimentation is conducted. The alternative fuel is the one with the highest adiabatic flame temperature. The program's output will also provide a close CDOM fuel proportion that will

limit experimental trial runs to avoid costly experiments.

OVERVIEW OF CDOM FUEL COMBUSTION REACTION THEORY

If fuels were burned in a furnace, such that no heat loss was incurred, then all the heat of combustion would be utilized for raising the temperature of the products of combustion. When combustion is completed under controlled conditions, the maximum amount of chemical energy from the fuel will have been converted into thermal energy, such that the temperature of the products of combustion will be at its maximum. This temperature is called the adiabatic flame temperature [1]. This will be the basis in determining the efficient CDOM proportion.

The combustion reactions of coal or diesel oil are discussed by the following authors Himmelblau [2], Horvath [3], Hsieh [4], Jones and Dugan [5], and Van Wylen and Sonntag [6]. Combustion takes place between the atoms of molecules of reactants, which are CDOM fuel and air resulting in the formation of molecules of products of combustion as gases formed during the burning of fuel. Thus, the fundamental combustion reaction equation is written on a molecular basis. The CDOM fuel used in the study is composed of $y\%$ Calatrava coal and $(1 - y)\%$ diesel oil. Calatrava

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coal is mined from Negros Occidental, Philippines and is considered to be a low quality fuel. It is ranked as sub-bituminous coal, which is known as black lignite [7]. Sub-bituminous is a low grade bituminous coal and contains a high percentage of moisture [8, 9]. Diesel oil as a mixture of hydrocarbons has a chemical name of dodecane with a chemical formula of $C_{12}H_{26}$ and a molecular weight of 170 kg/kg mole [1, 10]. The diesel oil used in this study is Grade 2 which is a distillate oil for general-purpose domestic heating [7, 8]. The diesel oil improves the quality of coal in the CDOM fuel and at the same time reduces the coal pollutants such as sulfur and ash [11]. Converting all the combustible elements from the ultimate analysis (mass fraction, f_{mi}) into mole fraction with total mass of CDOM fuel and molecular weight of individual components denoted by m_f and MW_i respectively.

Mass of Coal,

$$m_{coal} = ym_f \quad (1)$$

Mass of Diesel Oil,

$$m_{C_{12}H_{26}} = (1 - y)m_f \quad (2)$$

No. of kg moles,

$$n_i = \frac{f_{m_i}(m_{coal})}{MW_i} \quad (3)$$

Therefore, the number of kg moles of individual components in the reactants can be calculated as follows:

No. of kg moles of Carbon,

$$n_c = \frac{f_{m_c}(m_{coal})}{MW_C} \quad (4)$$

No. of kg moles of Hydrogen,

$$n_{H_2} = \frac{f_{m_{H_2}}(m_{coal})}{MW_{H_2}} \quad (5)$$

No. of kg moles of Oxygen,

$$n_{O_2} = \frac{f_{m_{O_2}}(m_{coal})}{MW_{O_2}} \quad (6)$$

No. of kg moles of Sulfur,

$$n_S = \frac{f_{m_S}(m_{coal})}{MW_S} \quad (7)$$

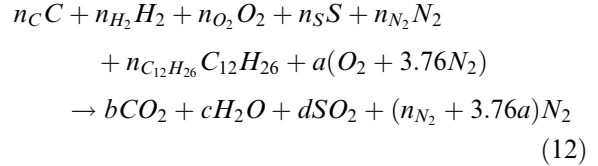
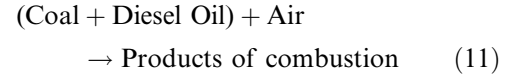
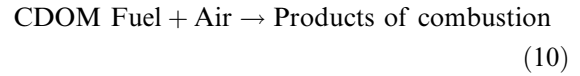
No. of kg moles of Nitrogen,

$$n_{N_2} = \frac{f_{m_{N_2}}(m_{coal})}{MW_{N_2}} \quad (8)$$

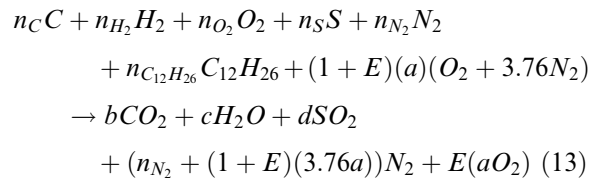
No. of kg moles of Diesel Oil,

$$n_{C_{12}H_{26}} = \frac{m_{C_{12}H_{26}}}{MW_{C_{12}H_{26}}} \quad (9)$$

Taken at a standard temperature of 25°K or 298°K and a pressure of 1 atm, the combustion reaction equation of CDOM fuel in 100% theoretical air can be written as:



In Equation (12), only a minimum amount of oxygen is included. In practice, this is not possible since it requires more oxygen than what is theoretically necessary to achieve complete combustion of the reactants. The excess air is needed because the fuel is of finite size and each droplet must be surrounded by more than the necessary number of oxygen molecules to assume oxidation of carbon, hydrogen, sulfur and other molecules in the fuel. Thus, the combustion reaction equation of CDOM fuel with the percent excess air (E) is given by:



By knowing the carbon, hydrogen, sulfur and oxygen balance in the above combustion equations, kg moles a, b, c, and d can be determined.

Algorithm formulation for the determination of the adiabatic flame temperature

Consider the energy diagram shown in Fig. 1 wherein CDOM fuel serves as the reactants and the gases formed are the products of combustion.

Applying the first law of thermodynamics:

$$H_R = H_P \quad (14)$$

where

H_R = total enthalpy of reactants, kJ

H_P = Total enthalpy of products, kJ.

The total enthalpy of reactants and products are determined as follows:

$$H_R = \sum n_i(h_{f_i}^o + \bar{c}_{p_i}(T_R - 298)) \quad (15)$$

$$H_P = \sum n_i(h_{f_i}^o + \bar{c}_{p_i}(T_P - 298)) \quad (16)$$

where

n_i = No. of kg moles of individual components in the reactants

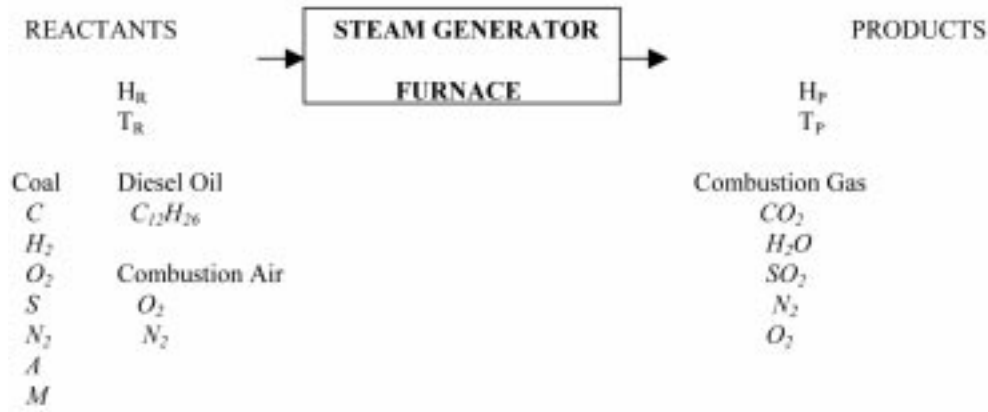


Fig. 1. Energy diagram showing the combustion of CDOM fuel.

n_j = No. of kg moles of individual components in the products

$h_{f_i}^o$ = Enthalpy formation of individual components in the reactants, kJ/kg mole

$h_{f_j}^o$ = Enthalpy formation of individual components in the products, kJ/kg mole

c_{p_i} = Molal specific heat at constant pressure of individual components in the reactants, kJ/kg mole °K

c_{p_j} = Molal specific heat at constant pressure of individual components in the products, kJ/kg mole °K

T_R = Reactants temperature, °K

T_P = Products temperature, °K.

The unknown coefficients expressed in kg mole on the reactants and products of Equation (13) may be determined by applying the law of conservation of mass to each reactants and products.

C balance:

$$b = n_C + n_{C_{12}H_{26}} \quad (17)$$

H₂ balance:

$$c = n_{H_2} + n_{C_{12}H_{26}} \quad (18)$$

S balance:

$$d = n_S \quad (19)$$

O₂ balance:

$$a = b + \frac{c}{2} + d - n_{O_2} \quad (20)$$

Equation (13) can be simplified further into:

$$(n_C C + n_{H_2} H_2 + n_{O_2} O_2 + n_S S + n_{N_2} N_2 + n_{C_{12}H_{26}} C_{12}H_{26}) + g(O_2 + 3.76N_2) \rightarrow bCO_2 + cH_2O + dSO_2 + eN_2 + fO_2 \quad (21)$$

The coefficients e, f and g can be determined using the following equations below:

$$e = n_{N_2} + (1 + E)(3.76a) \quad (23)$$

$$f = E(a) \quad (23)$$

$$g = (1 + E)(a) \quad (24)$$

For the reactants:

$$\begin{aligned} H_R = & n_C(h_{f_C}^o + \bar{c}_{p_C}(T_R - 298)) \\ & + n_{H_2}(h_{f_{H_2}}^o + \bar{c}_{p_{H_2}}(T_R - 298)) \\ & + n_{O_2}(h_{f_{O_2}}^o + \bar{c}_{p_{O_2}}(T_R - 298)) \\ & + n_S(h_{f_S}^o + \bar{c}_{p_S}(T_R - 298)) \\ & + n_{N_2}(h_{f_{N_2}}^o + \bar{c}_{p_{N_2}}(T_R - 298)) \\ & + n_{C_{12}H_{26}}(h_{f_{C_{12}H_{26}}}^o + \bar{c}_{p_{C_{12}H_{26}}}(T_R - 298)) \\ & + g(h_{f_{O_2}}^o + \bar{c}_{p_{O_2}}(T_R - 298)) \\ & + g(3.76)(h_{f_{N_2}}^o + \bar{c}_{p_{N_2}}(T_R - 298)) \end{aligned} \quad (25)$$

The molal specific heat at constant pressure of the individual components of reactants expressed in kJ/kg mole °K are:

$$\bar{c}_{p_C} = 11.193 + 1.096\theta_R - 48.95\theta_R^{-2} \quad (26)^{[2]}$$

$$\begin{aligned} \bar{c}_{p_{H_2}} = & 56.505 - 701.74\theta_R^{-0.75} \\ & + 1165\theta_R^{-1} - 560.7\theta_R^{-1.5} \end{aligned} \quad (27)^{[6]}$$

$$\begin{aligned} \bar{c}_{p_{O_2}} = & 37.432 + 0.020102\theta_R^{1.5} - 178.57\theta_R^{-1.5} \\ & + 236.88\theta_R^{-2} \end{aligned} \quad (28)^{[6]}$$

$$\bar{c}_{p_S} = 15.2 + 2.68\theta_R \quad (29)^{[1]}$$

$$\begin{aligned} \bar{c}_{p_{N_2}} = & 39.060 - 512.79\theta_R^{-1.5} + 1072.7\theta_R^{-2} \\ & - 820.40\theta_R^{-3} \end{aligned} \quad (30)^{[6]}$$

$$\bar{c}_{p_{C_{12}H_{26}}} = 36.35 + 37.23\theta_R \quad (31)^{[4]}$$

where: $\theta_R = T_R/100$; T_R in °K

For the products:

$$\begin{aligned} H_P = & b(h_{f_{CO_2}}^o + \bar{c}_{p_{CO_2}}(T_P - 298)) \\ & + c(h_{f_{H_2O}}^o + \bar{c}_{p_{H_2O}}(T_P - 298)) \\ & + d(h_{f_{SO_2}}^o + \bar{c}_{p_{SO_2}}(T_P - 298)) \\ & + e(h_{f_{N_2}}^o + \bar{c}_{p_{N_2}}(T_P - 298)) \\ & + f(h_{f_{O_2}}^o + \bar{c}_{p_{O_2}}(T_P - 298)) \end{aligned} \quad (32)$$

The molal specific heat at constant pressure of the individual components of the products expressed in kJ/kg mole °K are:

$$\bar{c}_{p_{CO_2}} = -3.7357 + 30.52\theta_p^{0.5} - 4.1034\theta_p + 0.024198\theta_p^2 \quad (33)^{[6]}$$

$$\bar{c}_{p_{H_2O}} = 143.05 - 183.54\theta_p^{0.25} + 82.751\theta_p^{0.5} - 3.6989\theta_p \quad (34)^{[1]}$$

$$\bar{c}_{p_{SO_2}} = 50.22 + 0.455\theta_p + -11072\theta_p^{-2} \quad (35)^{[1]}$$

$$\bar{c}_{p_{N_2}} = 39.060 - 512.79\theta_p^{1.5} + 1072.7\theta_p^{-2} - 820.40\theta_p^{-3} \quad (36)^{[1]}$$

$$\bar{c}_{p_{O_2}} = 37.432 + 0.0020102\theta_p^{1.5} - 178.57\theta_p^{1.5} - 178.57\theta_p^{-1.5} + 236.88\theta_p^{-2} \quad (37)^{[1]}$$

where:

$$\theta_p = T_p/100; T_p \text{ in } ^\circ\text{K}$$

PROGRAM DEVELOPMENT AND IMPLEMENTATION

The program was developed using HyperText Markup Language (HTML[®]) and JavaScript[®] for Microsoft Internet Explorer[®] 5.0 format, which facilitates the development of Internet and Windows-based packages. Scripting methods were adopted for ease of coding, portability (due to implementation on different Internet web browsers), faster and reliable data acquisition. The program design phase were as follows:

- Designing of the user interface.
- Scripting the algorithms and functions to the developed program.
- Writing miscellaneous code for the evaluation and validation of the user data input.
- Testing and debugging of the program for possible errors.
- Design review implementation for possible optimization of the scripted codes.
- Finalization and implementation of the developed program.

As discussed previously:

$$H_R \text{ is known, } H_P = H_R \text{ and } H_P = f(T_P) \quad (38)$$

The absolute temperature of the products or adiabatic flame temperature (T_P) cannot be solved directly. T_P will be solved by numerical methods such that ideally:

$$R = H_R - H_P = 0 \quad (39)$$

With a tolerable range of: $0 \leq R \leq 0.00001$.

Considering an initial temperature of products (T_P), R can be calculated using Equation (39). If R

exceeds the tolerable range, then (T_P) will be adjusted using the proportional integral derivative (PID) principle such that:

$$T'_R = T_P + 0.001(R/10) \quad (40)$$

where:

T'_R = adjusted temperature of products, °K
 T_P = absolute temperature of products for initial iteration = 298 °K
 0.001(R/10) = increment value.

With the adjusted temperature of the products (T'_R), the developed program will compute again for $\bar{c}_{p_{CO_2}}$, $\bar{c}_{p_{H_2O}}$, $\bar{c}_{p_{SO_2}}$, $\bar{c}_{p_{N_2}}$, $\bar{c}_{p_{O_2}}$ and H_R and H_P using Equations (33) to (38) until R falls in the tolerable range. The flow chart for the developed computer program is shown in Fig. 2.

The computer program requires the user to input the following data.

- CDOM fuel data:
 - Total mass of CDOM fuel, m_f kg
 - Percent coal in CDOM fuel, y , %
 - Percent Diesel oil in CDOM fuel, $(1 - y)$ %
- Ultimate analysis of coal:
 - Percent carbon, C %
 - Percent hydrogen, H₂ %
 - Percent oxygen, O₂ %
 - Percent sulfur, S %
 - Percent nitrogen, N₂ %
 - Percent ash, A %
 - Percent moisture, M %
- Combustion air condition:
 - Percent Excess Air, E %
 - Absolute temperature of reactants, T_R °K

After which, the developed program will compute for the absolute temperature of the product or adiabatic flame temperature (T_P) using numerical methods.

THE DEVELOPED PROGRAM EVALUATION

In running the program, the ultimate analysis of the Philippine Calatrava coal (Table 1) CDOM desired fuel proportion and the total mass of the fuel were inputted. The inputted data will be verified for errors by the program's algorithm. If errors were found, a halt in operation prompts the user to check the inputted values as shown in Fig. 3.

If no error incurred, the adiabatic flame temperature (T_P) will be computed. Table 2 shows a sample output of the adiabatic flame temperature for different CDOM fuel proportions at 20% excess air.

Theoretical calculations showed that the percentage of coal in the CDOM fuel sample is inversely proportional to the adiabatic flame temperature. The addition of more coal in the mixture further lowers the adiabatic flame temperature due to the low heating value of the coal. It is shown also in

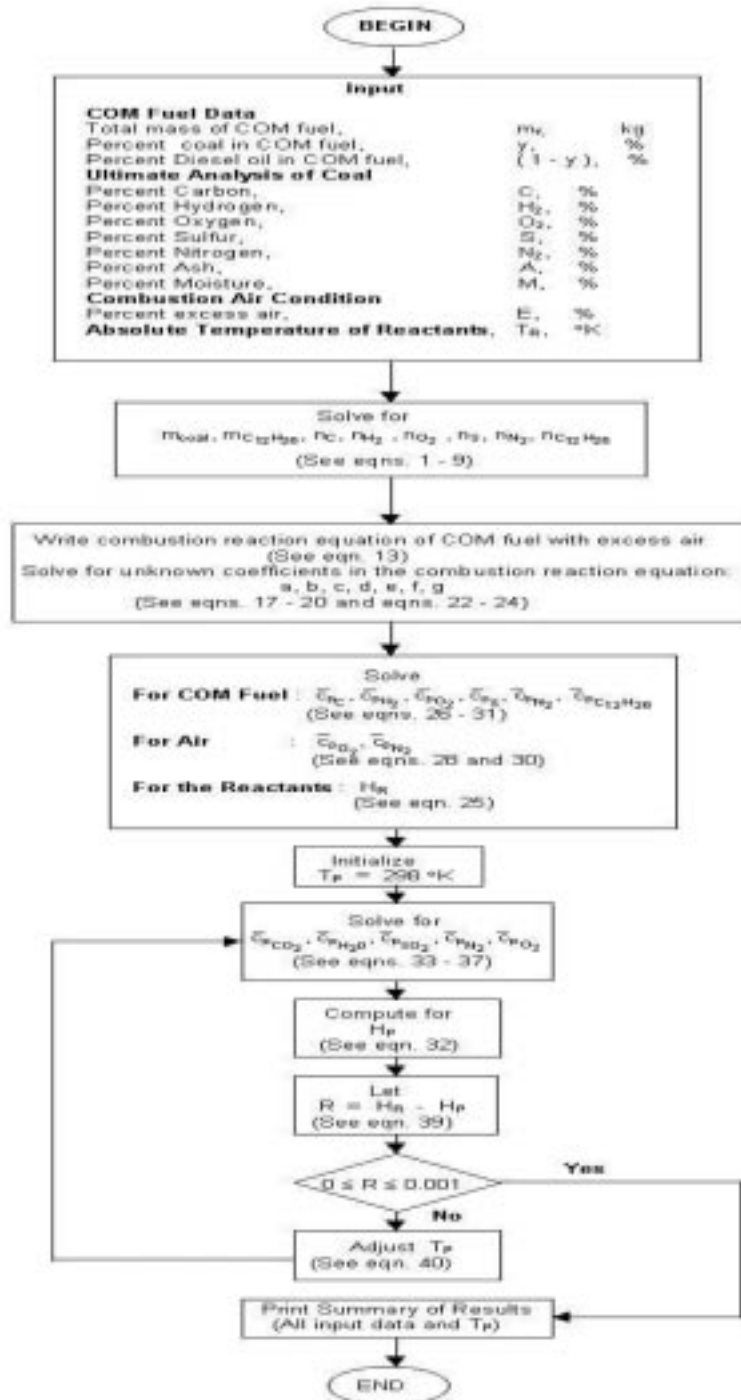


Fig. 2. Flowchart for writing the computer program for determining the adiabatic flame temperature from the system.

Table 1. Ultimate analysis of the Philippine coal

<i>Calatrava coal</i>	
Components	f_{mi} , %
Carbon, C	53.34
Hydrogen, H ₂	5.60
Oxygen, O ₂	10.79
Sulfur, S	0.65
Nitrogen, N ₂	1.40
Ash, A	11.30
Moisture, M	16.92
Total	100.00

Table 2. Adiabatic flame temperature of CDOM fuel samples based on system of equations at 20% excess air

<i>CDOM fuel proportion</i>	<i>Adiabatic flame temperature, T_P °K</i>
5% coal—95% diesel oil	2122.773
10% coal—90% diesel oil	2099.188
15% coal—85% diesel oil	2075.560
20% coal—80% diesel oil	2051.883

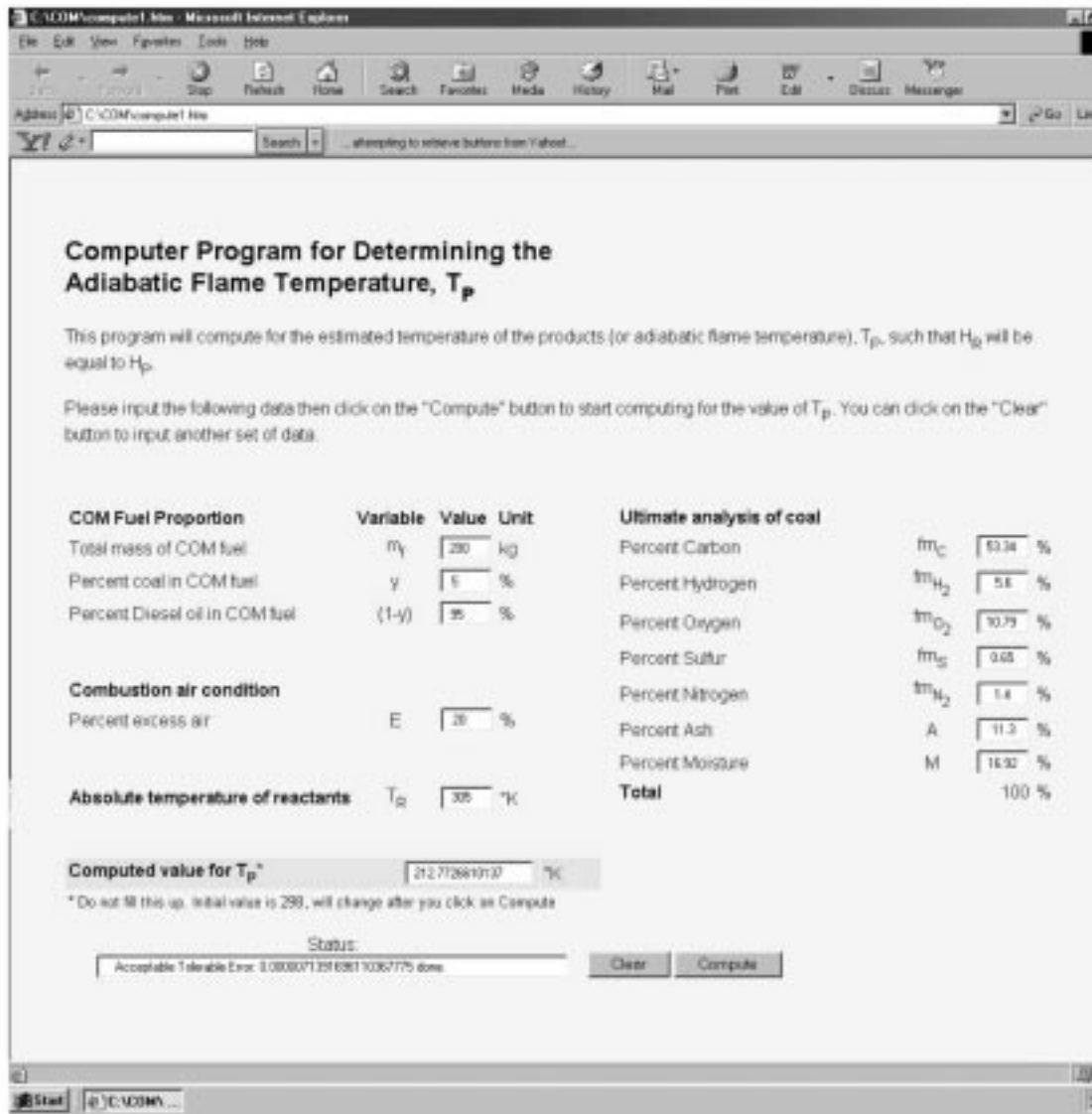


Fig. 3. Developed computer-assisted program user's interface: (a) interactive computer program for user data input and (b) activated warning dialogue boxes to prompt the user for input data errors.

Table 2, that a 5% coal—95% diesel oil concentration has the highest adiabatic flame temperature, which corresponds also to the heating value of the Philippine Caltrava CDOM fuel proportion validated by the actual experimentation discussed in the succeeding section, making it the most desirable alternative fuel for diesel oil. Figure 3 shows the summary of the results displayed on screen to aid actual experimentation.

ACTUAL EXPERIMENTATION AND DISCUSSION OF RESULTS

During the actual experimentation, the students prepared different proportions of CDOM fuel samples. The proportions of CDOM fuel samples were based on the output predicted by the program. Experimental procedures were based on the recommendations of Bajor and Trass [12], Capes and

Darcovich [13], and Mehrotra, Sastry and Morey [14]. The properties of diesel oil and CDOM fuel samples were determined based on American Society of Testing Materials (ASTM) Test Standards.

- ASTM D482–46: Determination of Ash Content, %A
- ASTM D524–42: Determination of Carbon Residue, %C_R
- ASTM D93–46: Determination of Flash Point Temperature, FP
- ASTM D240: Determination of Higher Heating Value, HHVS
- ASTM D1292: Determination of Specific Gravity and Density, SG_S
- ASTM D129: Determination of Sulfur Content, %S
- ASTM D88–44: Determination of Viscosity, μ_S
- ASTM D96–47: Determination of Water, %H₂O and Sediments, %Sed

Table 3 is a summary of the different properties of fuel samples gathered during experimentation. It shows that the selection of the appropriate alternative CDOM fuel for diesel oil can be based on the actual experimentation through the determination of the following fuel properties, namely: ash content, carbon residue, flash point temperature, specific gravity and density, sulfur content, viscosity, water and sediments and higher heating value. A 5% coal—95% diesel oil CDOM fuel proportion with a pulverized coal size of 200 mesh has similar properties to that of diesel oil making it a suitable alternative fuel to diesel oil. The same results were achieved considering the system of equations formulated and the computer-assisted program developed.

INTEGRATION OF THE DEVELOPED PROGRAM TO EXPERIMENTAL LABORATORY WORK

The developed program for the determination of the most efficient coal-diesel oil mixture (CDOM)

fuel proportion as alternative fuel to diesel oil is being used by the senior mechanical engineering students of De La Salle University in their Fuels and Combustion Laboratory classes. The general strategy in implementing the program, initially, is that the fuel combustion reaction theories are taught in the Combustion Engineering lecture subject of about forty (40) students. After the discussion of the principles, sample problems are illustrated and the students are given exercises to work on. With the complicated problems, the students experienced tedious and time-consuming manual computations. In the laboratory proper, the students are divided into two classes. Each class has five groups with four members per group and a brief demonstration of the developed program will be conducted. Through this developed computer program it will aid students with ease in the computation of problems encountered in the lecture subject. The results determined by the program will be the basis of experimentation. With the introduction of the program, the students were able to analyze more sample problems and established well-criticized experimental reports. Time-consuming manual computations were minimized and more time devoted to the laboratory experiments and investigation. The effectiveness of the teaching approach regarding the integration of the computer program in the laboratory exercise were satisfactory as it was closely observed by the instructor in the evaluation of the student's data analysis.

CONCLUSION

Based on the feedback of the faculty handling the subject, the developed computer-assisted program has significantly improved the quality of the laboratory work of the students. They were able to come up with results closely similar to the computer program compared with the actual

Table 3. Summary of fuel sample properties

Fuel Sample ()	% A	% C _R	FP, °C	HHV _g J/g	SG _S	% S	μ _g (cP) 90 °C	% H ₂ O	% Sed.
DIESEL OIL	0.02	0.119	84	45257.27	0.825	1.05	2.068	0.1	0.01
CDOM FUEL									
–50 + 100 Mesh									
5% coal—95% diesel oil	5.43	0.871	88	41105.72	0.771	1.35	6.845	2.53	24.4
10% coal—90% diesel oil	6.78	1.263	94	38765.08	0.776	1.52	7.976	3.25	30.1
15% coal—85% diesel oil	8.45	1.638	96	30706.27	0.782	1.59	10.938	4.91	35.3
20% coal—80% diesel oil	10.72	1.972	98	26764.53	0.784	1.62	13.616	5.18	38.5
–100 + 200 Mesh									
5% coal—95% diesel oil	4.84	0.318	90	43554.33	0.741	1.54	4.628	1.13	17.26
10% coal—90% diesel oil	5.13	0.983	96	4221.77	0.754	1.63	5.223	2.18	22.36
15% coal—85% diesel oil	7.85	1.102	98	32990.75	0.761	2.13	7.143	2.83	28.1
20% coal—80% diesel oil	9.36	1.812	102	29674.05	0.782	2.33	8.78	3.12	32.52
–200 Mesh									
5% coal—95% diesel oil	3.23	0.196	94	44195.37	0.722	1.93	2.46	0.78	12.46
10% coal—90% diesel oil	4.18	0.826	98	42909.1	0.739	2.38	4.167	1.87	18.7
15% coal—85% diesel oil	6.52	1.057	110	34415.32	0.752	2.54	5.7	1.98	22
20% coal—80% diesel oil	8.67	1.513	115	30413.84	0.774	2.9	7.46	2.63	30.62

experimentation. The paper has explained in detail how the underlying principles in carrying out the tedious manual computation. Considerable amounts of time were saved with the introduction of the developed computer program, thus more time was devoted in the experimental data analysis rather than its generation. The experimental reports submitted shows that the students have become more in-depth in their analysis and more

critical in their approach. However, it must be noted that the developed computer-assisted program is not meant to replace the traditional methods of teaching but rather to supplement them. With the continuous advancement in energy technology, engineering students should be prepared to the challenges in their professional careers particularly in the search of alternative fuel that has less environmental risk.

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Archie B. Maglaya is a full professor of the Department of Mechanical Engineering (Graduate and Undergraduate Programs) of De La Salle University-Manila, Philippines. He holds the California Manufacturing Company Inc. Distinguished Professorial Chair in Mechanical Engineering. He obtained his Bachelor's Degree in Mechanical Engineering from FEATI University-Manila, Master's Degree in Engineering Education Major in Mechanical Engineering from De La Salle University-Manila and Doctorate Degree in Technology (Academic Excellence Award) from Technological University of the Philippines. He had been a research fellow in the field of production engineering and involved in engineering design and design of production equipment at Loughborough University of Technology, Leicestershire, England and on cryogenics at Tokyo Institute of Technology, Japan. His research interests are in the area of pollution control and environmental protection, energy and alternative fuels, equipment design and fabrication and engineering education. He is a Life Member of the Philippine Society of Mechanical Engineers (PSME), Founding Member and Director of the Philippine Institute of Mechanical Engineering Educators (PIMEE), Associate Member of the National Research Council of the Philippines (NRCP), Associate Member of the American Society of Mechanical Engineers (ASME) New York, USA and Senior Member of the Society of Manufacturing Engineers (SME) Dearborn, Michigan, USA.