

Flame Temperature and Species Calculations with an Excel/VBA Computer Code

David G. Lilley

Lilley & Associates, 7221 Idlewild Acres, Stillwater, Oklahoma 74074

Email: DGL@firedynamics.com

As a contribution to applied combustion calculations with and without dissociation of H₂O and CO₂, a simple, easy-to-use calculation procedure has been developed that permits rapid generation of general fuel-air and fuel-oxygen combustion with many parameter variations. Many fuels and mixtures, including municipal solid wastes, plastic and non-plastic, may be easily handled in the developed computer code. It is written in Excel/VBA and the program calculations are with immediate graphics of the parameter effects on the results, thus permitting an extensive range of parameter effects to be quickly investigated and assessed. The very-general fuel is specified by way of its C-H-O-N-S content. Over 100 standard fuels are in the data base for immediate calculations. Percentages of these may be specified easily so that several of them (and/or new fuels added by the user) are combined for a single calculation. Additional water content is easily specified by the user. The "air" is specified by way of the volume percent of oxygen, and the other component of "air" (nitrogen and/or carbon dioxide) is specified by the user. So also is the temperature of each inlet, the inlet fuel and "air" streams. The methodology and computer code takes as input also the equivalence ratio.

A computer code is described which calculates the adiabatic flame temperature under the following user choices:

- Type of fuel (CHONS amounts and heating value on a mass basis specified)
- Different equivalence ratios
- Type of oxidant (air or oxygen)
- With and without limited dissociation of CO₂ and H₂O, and more detailed dissociation reactions
- With "air" as the oxidant, the volume fraction of oxygen is specified
- The inlet temperatures of the fuel and oxidant streams individually are specified

Two types of results are generated: (a) the adiabatic flame temperature with the equilibrium product species both with and without dissociation; and (b) with the products temperature specified then the heat transfer inside the combustor is calculated, on the basis of products both with and without dissociation. In both these cases, the calculation automatically includes combustion in "air" and oxygen alone.

The computer code is very user friendly, with automatic nested loops for parameter variation and automatic generation of graphs, which are particularly useful in assessing the particular process under consideration.

I. Introduction

It is often necessary to know the adiabatic flame temperature and corresponding product species composition in a chemically reacting system. However, experimentation to determine this is very delicate, costly, and time consuming. For this reason, theoretical calculations are preferred, where results of calculations from a model can be

checked against a limited set of experimental data. Then extrapolations can be made to other conditions of interest. The effect of each parameter on the results may then be deduced theoretically. However, the theoretical prediction of temperature and product species amounts are neither easy nor quick, and available computer codes usually do not have the ease and range of application desired. Standard undergraduate thermodynamics courses present chemical reaction expressions and apply energy balance methods. Both dissociated and non-dissociated product species are also considered. Techniques are generally presented which permit the deduction of the flame temperature and the relative amounts of the individual species in the reaction products. But, the methods used by and large require 'trial and error' iterative hand calculations, with student interpolation of values from thermodynamic tables and/or the assumption of known constant specific heats.

A calculation procedure is described that permits rapid calculation of fuel-air combustion with a very large range of general fuels and conditions covering those for the use of alternative fuels in advanced power generation. Calculations are made via Excel/VBA with immediate graphics of the parameter effects on the results. A large range of useful results have been generated. Parameter variations include:

1. Type of fuel amounts specified via C-H-O-N-S amounts and/or molar (volume) or mass fractions of multi-component fuels
2. Different equivalence ratios
3. Type of oxidant (air or oxygen)
4. With and without limited dissociation of CO_2 and H_2O , and more detailed dissociation reactions
5. With "air" as the oxidant, the volume fraction of oxygen is specified, the other component of air may be nitrogen or carbon dioxide or a combination of the two, and an amount of water may accompany the inlet fuel and oxidant streams
6. The inlet temperatures of the fuel and oxidant streams individually are specified

The most complicated case required nested half-interval searches for temperature and species. Results show the accuracy, robustness and versatility of the code, and its ease of applicability to realistic combustion situations. Useful illustrative calculations were also given for municipal solid wastes, and their adiabatic flame temperature and, alternatively, the combustor internal heat transfer when the exit temperature is known. Current application is to a vast range of additional reaction features.

Significant energy savings, higher and uniform thermal field, lower pollution, and smaller size of equipment for a range of furnace applications – these have all been demonstrated via recent advances on High Temperature Air Combustion (HiTAC) or flameless oxidation. Burning of alternative fuels, and prospects of energy recovery from wastes and associated HiTAC technologies, are discussed in Tsuji et al (2003) and Gupta and Lilley (1999 and 2003). The thermal and chemical behavior of these flames depend on the precise fuel composition, preheat temperature, and oxygen concentration of air. Waste heat from a furnace using HiTAC is retrieved and introduced back into the furnace using a regenerator. These features help save energy, which subsequently also reduce the emission of CO_2 (greenhouse gas) to the environment. Flames with high temperature air provide significantly higher and more uniform heat flux than normal air, which reduces the equipment size or increases the process material throughput for the same size of equipment. The high temperature air combustion technology can provide significant energy savings (up to about 60%), downsizing of the equipment (about 30%), and pollution reduction (about 25%).

In the incineration of municipal solid waste for energy production and minimal pollution, new "high temperature air combustion" HiTAC technologies are evolving. As a contribution to this area of current research interest, a calculation procedure has been developed that permits rapid generation of general fuel-air combustion with many parameter variations. It is written in Excel/VBA and the program calculations are with immediate graphics of the parameter effects on the results, thus permitting an extensive range of parameter effects to be quickly investigated and assessed. The very-general fuel is specified by way of its C-H-O-N-S content. Additional water content is easily specified. The "air" is specified by way of the volume percent of oxygen, and the other component of "air" (nitrogen and/or carbon dioxide) is specified by the user. So also is the temperature of each inlet, the inlet fuel and "air" streams. The methodology and computer code takes as input also the equivalence ratio. Then, results of adiabatic flame temperature are calculated along with the equilibrium product species both with and without dissociation. Alternatively, the products temperature may be specified and the heat transfer in the combustor is then calculated. The computer code is very user friendly, with automatic nested loops for parameter variation and

automatic generation of graphs, which are particularly useful in assessing the particular process under consideration. The application now is to incineration of municipal solid waste for energy production and minimal pollution. The waste may consist of a variety of specified components, including plastics and non-plastics, cellulose, cardboard, wood, etc. and the relative amounts are given as inputs.

II. Flame Temperature and Product Species Calculation

Typically, thermodynamics textbooks present the ideas of chemical reactions, dissociation, flame temperature, and product species; but the techniques given are often in a manner that is not computerizable. Often, even the computerized methods given lack generality and ease of use. On the other hand, combustion-oriented texts (for example, see Kuo (1986)) are not usually studied by engineering undergraduates or graduates who are not combustion specialists. Other texts concentrate on fuels, see Goodger (1975) and Odgers and Kretschmer (1986), and combustion aerodynamics and its applications, see Beer and Chigier (1972) and Gupta and Lilley (1985).

None of these texts give general computerized methods for finding the adiabatic flame temperature and product species amounts, including some degree of dissociation. Only advanced research reports (for example, Gordon and McBride (1971)) give very general computerized methods with a significant sophistication given to the dissociation aspects of the calculation. Some combustion-oriented texts do include methods and results of computerized calculations of flame temperature (see, for example, Borman and Ragland (1998) and Turns (2001)) and some texts include a computer code, see, for example, Turns (2001). None of them present easily computerizable flame temperature and species calculation methodologies, with and without dissociation, with oxidizer air alone and pure oxygen, that can be used easily and quickly by the practicing applied combustion engineer. The present objective is to present a useful Exce/VBA code that permits easily a wide range of calculations to be accomplished and graphed easily by the practical man.

A straightforward computer code has been developed and is now described which calculates the adiabatic flame temperature and product species amounts for general CHONS fuels. The program is named Adiabatic Flame Temperature Calculation (AFTC). It is useful for calculations within in a computational fluid dynamics reacting flow computation, and it is readily incorporated into undergraduate and graduate course studies. It is based on the methods of Goodger (1977) and Campbell (1979). The theoretical background and computational algorithms used in its development are presented. The parameters used are: fuel type, equivalence ratio, reactant temperatures and pressure, type of oxidant and air composition, and inclusion of dissociation effects. This work builds on previous papers, Lilley (2004) and Olinger and Lilley (2004a and b, and 2005a). Results are given for a range of input parameters so as to illustrate the versatility of the computer program. Associated results applicable to the new technology of high temperature air combustion are given in an associated paper; see Olinger and Lilley (2005b).

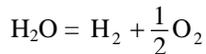
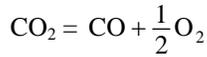
The standard expression for general fuel-air combustion is:



The right hand side represents the major combustion product species. Without dissociation, the n_i -values are readily specified (the so-called "cold" products of combustion). With dissociation, the more detailed n_i -values are deducible via a half-interval search technique at a given temperature. Additionally, more complex dissociated product species may occur, including O, H, OH, and NO.

For an oxidizer of standard dry air, $f = 3.762$. This occurs as standard dry air consists of 21 percent oxygen by volume, and nitrogen is reckoned to provide the other 79 percent. These values correspond to 23.2 percent oxygen by mass and 76.8 percent nitrogen by mass. The value of m is determined from the burning conditions (the amount of oxidant supplied relative to the amount of fuel supplied). It strongly controls the number of moles of product species (n_1, n_2, \dots, n_7) by restricting complete fuel combustion of the fuel or by adding extra oxidizer for dissociation.

Dissociation reactions absorb thermal energy, thus lowering the product's temperature. One of the simplest and most effective assumptions about dissociation is that at high temperatures some of the CO_2 in the product stream will dissociate into CO and O_2 and some of the H_2O in the product stream will dissociate into H_2 and O_2 . These primary reactions are represented by:



The degree of dissociation is dependent on both the combustion pressure and temperature, and is such that the molar (volume) fractions obey the laws of mass action.

Appendix A provides detailed information about the iterative solution procedure, with half-interval searches for temperature and species amounts. The methodology for solution of these equations for the adiabatic flame temperature and product species, with and without this limited dissociation, has been described in detail by Lilley (2004) and further development and application by Olinger and Lilley (2004a and b, and 2005a and b). Half interval search procedures in nested loops are used for both temperature and species calculations, using fitted curves for temperature variation of enthalpy and partial pressure chemical equilibrium constants. Energy balance and species conservation checks ensure convergence of the AFTC code. Problem specification, data input, and operation of the computer code are therefore not further discussed here.

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A. AFTC -Composite

The first version of AFTC, called *AFTC-composite*, creates a composite fuel by merging a list of user selected fuels. The program allows the user to choose from an array of 200 fuels that are already on the spreadsheet with CHONS composition and lower heating value. The chosen fuels are automatically merged into a single fuel with correct representation of its chemical formula and heating value, and the flame temperature calculations ensue from this. In this way, the new fuel's properties are the respective proportional sums from that of each component fuel.

To aid in data generation, this computer program includes additional nested loops for parameter variations. The inner loop runs the basic AFTC code seven times, each time changing the reactant temperatures as per the user's input. Furthermore, the iterated steps are displayed on succeeding pages within the spreadsheet, with each page showing convergence for each case. The outer loop then runs each of these inner loops over a series of seven oxygen percentages in the air, by volume. In this way, forty-nine sets of data for a given pressure and equivalence ratio may be generated quickly and easily, with seven automatically generated graphs.

B. AFTC-Multifuel

The second version of AFTC, called *AFTC-multifuel*, keeps the core loop structure of AFTC, and expands upon it to handle many different fuels. The same fuel listing used in the Composite program is used in this variation. Temperature and products are calculated for each fuel in turn, allowing automatic, fast generation of eight graphs and useful tables. These permit immediate comparison of different fuels and properties, such as how the adiabatic flame temperature varies with the carbon number of a fuel, equivalence ratio, inlet reactant (fuel and "air") temperatures, etc.

III. Results and Discussion

A. Comparison with Other Methods

Other methods exist that may offer a more direct solution to the above equations, but at the cost of guaranteed convergence, Campbell (1979). One such method for solving the flame temperature and product composition is to use a Newton-Raphson iteration procedure. This is the method used in both the well-known programs by Turns (2001) and Gordon-McBride (1971). It is also implemented in Ferguson and Kirkpatrick (2001). In addition to the dissociated species accounted for in AFTC, these programs also account for H, NO, O, OH, and N. Goodger (1977) also gives temperature predictions. The present code has been run for a variety of situations and compared very favorably, typically less than a one percent difference in temperature. The results for Turns were obtained by running the program. Results for Gordon-McBride were cited in Glassman (1987). Results for Goodger (1977) and

Ferguson and Kirkpatrick (2001) are from their respective books. Table 1 displays the adiabatic flame temperature found by each program. Table 2 then recalculates the results of Table 1 to give each program's percent difference in temperature, relative to the present AFTC calculations.

Adiabatic flame temperature values for a variety of fuels found in the above works are listed in Table 1. Furthermore, Table 2 provides the percent differences in these temperatures. In all cases where data was available, the percent difference in each work's results is less than two percent. This corresponds to a temperature difference of approximately 30K, despite the different dissociation constraints. Except for Gordon and McBride's result for methane, 1.68%, AFTC showed less than one percent difference with all the programs for the standard hydrocarbons. This covers the range from the high temperature acetylene to the relatively low temperature methane. Additionally, the oxygen bearing and nitrogen bearing fuels see an extremely small temperature difference across the different programs. Methanol has a maximum difference of 0.63% and cyanogen has maximum difference of only 0.29%. Finally, hydrogen and carbon monoxide exhibit the greatest disparity across the different programs, both on the order of 1.5%.

There are three primary reasons for these slight differences. We take standard air consisting of 21% oxygen, there are 3.762 moles of nitrogen for every mole of oxygen in the air. Some codes use 20.9% oxygen. Additionally, there are slightly different physical constants and different parametric curve-fits of enthalpy versus temperature. We use a simple three parameter curve over the temperature range 1600K to 6000K. And of course, each calculation method has to converge to an answer, but what degree of convergence is used. The precise specification is not well documented in the other methods mentioned here.

B. Comparison of General HC Fuels

After the comparison with other computer programs, AFTC was run for a variety of different fuels and equivalence ratios, the results of which are displayed at the end of this paper. For example, many fuels, grouped into acetylenes, paraffins, and olefins, are calculated for stoichiometric combustion. These results are given in Figure 1. The adiabatic flame temperature is graphed against the carbon number of the fuel. Notice all the curves, each representing a different class of fuels, converge to one temperature as the carbon number increases. This is justification for the common practice in industry of modeling complex fuels as composites of simpler fuels. After these results were displayed, the equivalence ratio was changed to fuel lean and fuel rich conditions. From Figures 2 and 3, one finds the temperatures are highest for nondissociated combustion. As the equivalence ratio shifts from unity, the temperature decreases.

C. Comparison of CHON Fuels

With AFTC run for basic HC fuels, the fuel listing was expanded to include fuels containing carbon and hydrogen, results of which are displayed in Figure 4. Once more, the dependency of the flame temperature, and thus dissociation, upon the carbon number is demonstrated. As the carbon number takes a larger fraction of the molecule, the flame temperatures approach a single value. Notice that these fuels have lower heat release on a mass basis than the HC-only fuels.

D. Municipal Solid Waste Fuels

The plastic/ versus non-plastic relative amounts in municipal solid waste has a dramatic effect on the heating value of the fuel, and the product species produced, and their adiabatic flame temperature or, alternatively, the amount of heat transferred internally in a furnace or boiler when the exit temperature is less than the adiabatic flame temperature. General results have been generated and discussed at length before, see Lilley (2004, 2008 and 2009) and Olinger and Lilley (2004a and b, and 2005a and b).

The composition of the waste varies significantly from source to source and also from season to season. Typical composition of the dry MSW is given in Table 3. The presence of moisture (which can vary from 10 to 66%) can have a significant influence on the heating value of the waste. Dry Municipal Solid Waste MSW has an approximate heating value of 16.2 MJ/kg (or equivalently 6,968 Btu/lb), see Table 4. As an example, a 10% increase in moisture will reduce the heating value of waste by about 1.67 MJ/kg (or equivalently 717 Btu/lb). The decrease in heating value (in Btu/lb) with the increase in moisture content can reasonably be estimated from $(6968 - 71.7x)$, where x is the moisture content in weight percent. The average moisture content in material depends on the material type. Food waste may have moisture content of about 70%, while plastic and leather have very low moisture content of about 2%. There are seasonal variations of the moisture and energy content of the wastes.

Therefore, the sorting of the material cannot only provide near uniform chemical composition but also energy content. A comparison of heating values of municipal waste with various other waste fuels and biomass is given in Table 4. The data shows that the energy content in the MSW is comparable with some wood material and wastes.

E. Calculations of Adiabatic Flame Temperature for Plastics and Non-Plastics

Figure 5 shows the adiabatic flame temperature of a variety of plastics and non-plastics burning in fuel lean, standard air, from 25% excess air to stoichiometric, represented by equivalence ratio ϕ from 0.8 to 1. As expected, the maximum flame temperatures occur at stoichiometric conditions, and decrease with a decreasing fuel concentration. Polystyrene (C_8H_8 , lower heating value of 39.75 MJ/kg of fuel) and cellulose ($C_6H_{10}O_5$, lower heating value of 16.12 MJ/kg of fuel) are used to represent plastic and non-plastic, because their values approximate typical values for all plastics and non-plastics. Adiabatic flame temperatures of composite fuels with different mass fractions of the representative plastic and non-plastic are also calculated, the results of which are shown in Figure 6 and Table 5. As expected, the maximum adiabatic flame temperature occurs at an equivalence ratio of one, and decrease with greater amounts of excess air, as ϕ reduces. Plastic/non-plastic mixtures are calculated for 100%(mass) plastic to 0%(mass) plastic, at intervals of 25%(mass). Notice that, the higher the plastic content, the higher the temperature, because of the higher heating value of the plastic-rich fuel. Also, it is seen that the curves are clustered towards the pure plastic case, indicating that the flame temperature is progressively more sensitive to changes in the non-plastic content, as that content becomes increasingly larger.

F. Calculations of Combustor Internal Heat Transfer versus Combustion Product Temperature for Plastics and Non-Plastics

In Figures 7 through 9, the internal heat transfer from the flame in the combustor region (of the combustion chamber, furnace or boiler) is calculated, on the basis that the combustor exit temperature is specified. Figure 7 is for a 1500K exit temperature, Figure 8 is for a 1000K temperature, and Figure 9 is for a 500K temperature. Each figure shows the heat transfer from the flame within the furnace as a function of the equivalence ratio. The same variety of fuel plastic/non-plastic mixtures as before is considered. Numerical results for Figures 7 through 9 are given in Tables 6 through 8, respectively. As expected, the heat transfer from the flame is highest (among the range of different fuels and equivalence ratios considered) for pure plastic burning at stoichiometric conditions. This is because the pure plastic at stoichiometric conditions would have had the highest flame temperature. Thus, when the exit temperature is reduced to the specified value, the amount of energy transferred internally is highest. Additionally, comparing the three figures and noting that the ordinate scale changes, the heat transferred from a flame increases as the specified combustion products temperature decreases. That is, the lower the exit temperature, the greater is the internal heat transferred from the flame. Concepts of the specific heat increasing with temperature, more so with greater oxygen and nitrogen content in the combustion products, give rise to why the slope of the lines becomes flatter as the exit temperature is reduced, that is, over Figures 7 through 9.

G. Pressure and Oxygen Fraction in "Air" Effects

Finally, after varying the equivalence ratio and fuel type, the flame temperature's dependence on the pressure and oxidizer were explored. Figure 10 consists of two flame temperature curves, one for dissociation and one for no dissociation. The first graph has a low pressure of half an atmosphere and serves to illustrate the increased dissociation at below average pressures. As the pressure is increased, the temperatures increase correspondingly. Despite this however, high pressures suppress dissociation, as can be seen in the 5atm and 10atm graphs. This is most clearly seen by noting that the high-pressure temperature curves are closer together than the low-pressure temperature curves. Furthermore, separation of the two curves is delayed until higher temperatures associated with increasing oxygen percents in the "air" occur, with higher temperatures and greater dissociation.

IV. Conclusions

A computer code has been developed using Excel/VBA to permit the rapid calculation of adiabatic flame temperatures and product species compositions for a large variety of easily specified fuel and air reactant conditions. An equilibrium combustion calculator such as AFTC can be a powerful aid to the power generation industry. The most complicated case required nested half-interval searches for temperature and species. Results show the accuracy, robustness and versatility of the code, and its ease of applicability to realistic combustion situations. Useful illustrative calculations were also given for municipal solid wastes, and their adiabatic flame temperature

and, alternatively, the combustor internal heat transfer when the exit temperature is known. Results are calculated immediately for the cases of "air" (with specified oxygen volume percentage) as the oxidant, with and without dissociation. Alternatively, the product temperature may be identified, and then the heat transfer in the combustor is calculated. In the user input section, the reaction is simply specified by way of the fuel's CHONS formula and its lower heating value, and the oxidizer's makeup. Once the equivalence ratio is set, a variety of calculations are generated automatically, covering a spectrum of initial parameters. Current application is to a vast range of additional reaction features.

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Table 1. Comparisons of the dissociated stoichiometric adiabatic flame temperature (K) as predicted by AFTC, Goodger (1977), Turns (2001), Ferguson and Kirkpatrick (2001), and Gordon and McBride (Glassman, 1987) in dry standard air

Comparison of Adiabatic Flame Temperatures (K)						
Fuel	Formula	AFTC	Goodger	Turns	F&K	G&M
Methane	CH ₄	2248	2247	2226	2227	2210
Propane	C ₃ H ₈	2274	2289	2267	2268	-
Heptane	C ₇ H ₁₆	2281	2298	2274	-	2290
Acetylene	C ₂ H ₂	2558	2583	2539	2540	-
Methanol	CH ₃ OH	2229	2243	2221	-	-
Hydrogen	H ₂	2419	2444	2382	2383	2400
Carbon Monoxide	CO	2364	2399	2383	-	2400
Cyanogen	C ₂ N ₂	2588	-	2594	2596	-

Table 2. Percent differences of the dissociated stoichiometric adiabatic flame temperature (K) as predicted by AFTC, Goodger (1977), Turns (2001), Ferguson and Kirkpatrick (2001), and Gordon and McBride (Glassman, 1987) in dry standard air

Percent Differences in Adiabatic Flame Temperature Calculations						
Fuel	Formula	AFTC	Goodger	Turns	F&K	G & M
Methane	CH ₄	0	-0.03	-0.97	-0.92	-1.68
Propane	C ₃ H ₈	0	0.67	-0.30	-0.26	-
Heptane	C ₇ H ₁₆	0	0.76	-0.30	-	0.40
Acetylene	C ₂ H ₂	0	0.99	-0.73	-0.69	-
Methanol	CH ₃ OH	0	0.63	-0.35	-	-
Hydrogen	H ₂	0	1.05	-1.52	-1.47	-0.77
Carbon Monoxide	CO	0	1.46	0.78	-	1.50
Cyanogen	C ₂ N ₂	0	-	0.21	0.29	-

Table 3. Characteristic Composition of the Dry Municipal Solid Waste

Component	Average Content (% weight)	Heating Value dry (Btu/lb)
Food waste	33.5	6,528
Paper, Cardboard	33.5	7,500
Plastics	9.2	14,000
Ferrous metal	7.8	300
Glass	5.8	250
Leather and rubber	4.8	13,000
Textiles and rags	3.7	7,652
Stones and ceramics	1.5	652
Nonferrous metals	0.2	13,000

Table 4. A Comparison of Heating Values of Municipal Solid Waste with other wastes, Refuse derived Fuels, Biomass and Fossil Fuels

Waste Type (Fuel)	Heating value (Btu/lb)	Heating value (MJ/kg)
Cellulose	7,300	17.00
Lignin	9,111	21.20
Wood (Pine)	9,600	22.30
Wood (Oak)	8,296	19.30
Coal (Sub-Bituminous)	11,729	27.30
Peat	8,237	19.20
Municipal Solid Waste (dry)	6,968	16.20
Municipal Solid waste (50% moisture)	3,380	7.90
Refuse derived Fuel (RDF)	7,942	18.50

Table 5. Adiabatic Flame Temperature (K) of Mass Mixtures of Plastics (P) and Non-Plastics (NP) vs. Equivalence Ratio

FLAME TEMPERATURE (K)		Fuel Equivalence Ratio				
		0.80	0.85	0.90	0.95	1.00
Mass Composition	100/0 mass P/NP	2116	2192	2255	2305	2340
	75/25 mass P/NP	2103	2177	2240	2289	2324
	50/50 mass P/NP	2084	2156	2218	2267	2300
	25/70 mass P/NP	2055	2126	2186	2234	2266
	0/100 mass P/NP	2008	2074	2132	2178	2208

Table 6. Heat Transfer From Flame at 1500K vs. Equivalence Ratio for Various Mass Mixtures of Plastic/Non-Plastic

HEAT RELEASED (MJ/kg of fuel)		Fuel Equivalence Ratio				
		0.80	0.85	0.90	0.95	1.00
Mass Composition	100/0 mass P/NP	14.9	16.2	17.3	18.4	19.3
	75/25 mass P/NP	12.5	13.6	14.6	15.4	16.2
	50/50 mass P/NP	10.1	11.0	11.8	12.5	13.2
	25/70 mass P/NP	7.7	8.4	9.0	9.6	10.1
	0/100 mass P/NP	5.3	5.8	6.3	6.7	7.0

Table 7. Heat Transfer From Flame at 1000K vs. Equivalence Ratio for Various Mass Mixtures of Plastic/Non-Plastic

HEAT RELEASED (MJ/kg of fuel)		Fuel Equivalence Ratio				
		0.80	0.85	0.90	0.95	1.00
Mass Composition	100/0 mass P/NP	25.9	26.7	27.3	27.9	28.4
	75/25 mass P/NP	22.0	22.6	23.2	23.6	24.1
	50/50 mass P/NP	18.0	18.5	19.0	19.4	19.8
	25/70 mass P/NP	14.1	14.5	14.8	15.1	15.4
	0/100 mass P/NP	10.1	10.4	10.7	10.9	11.1

Table 8. Heat Transfer From Flame at 500K vs. Equivalence Ratio for Various Mass Mixtures of Plastic/Non-Plastic

HEAT RELEASED (MJ/kg of fuel)		Fuel Equivalence Ratio				
		0.80	0.85	0.90	0.95	1.00
Mass Composition	100/0 mass P/NP	36.0	36.2	36.4	36.6	36.7
	75/25 mass P/NP	30.6	30.8	31.0	31.1	31.2
	50/50 mass P/NP	25.3	25.4	25.5	25.6	25.7
	25/70 mass P/NP	19.9	20.0	20.1	20.2	20.3
	0/100 mass P/NP	14.5	14.6	14.7	14.7	14.8

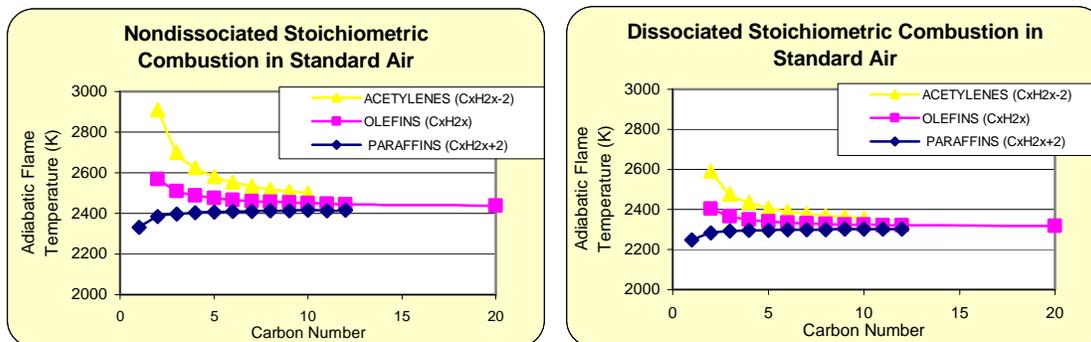


Figure 1. Stoichiometric Adiabatic Flame Temperature as a Function of the Fuel Carbon Number

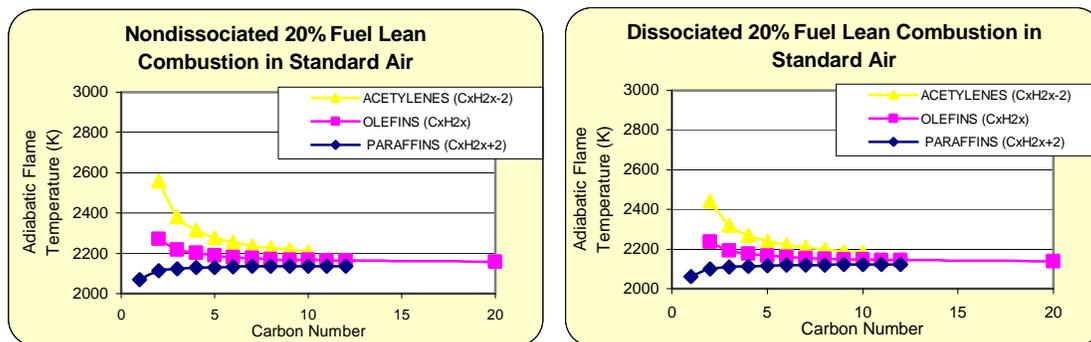


Figure 2. 20% Fuel Lean Adiabatic Flame Temperature as a Function of the Fuel Carbon Number

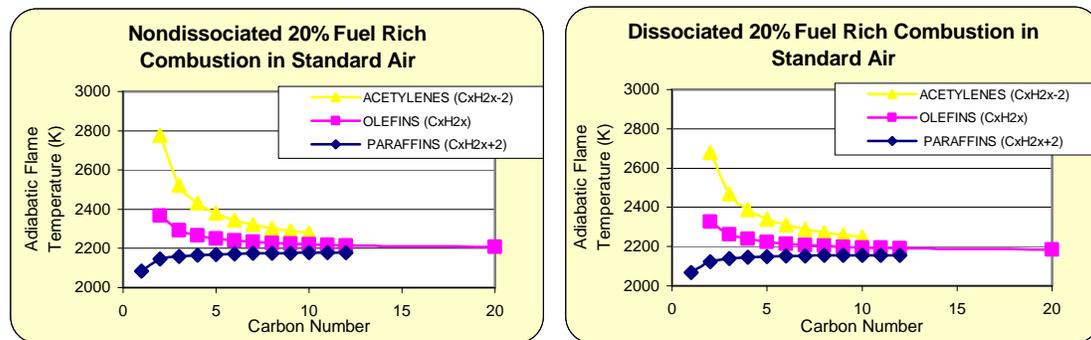


Figure 3. 20% Fuel Rich Adiabatic Flame Temperature as a Function of the Fuel Carbon Number

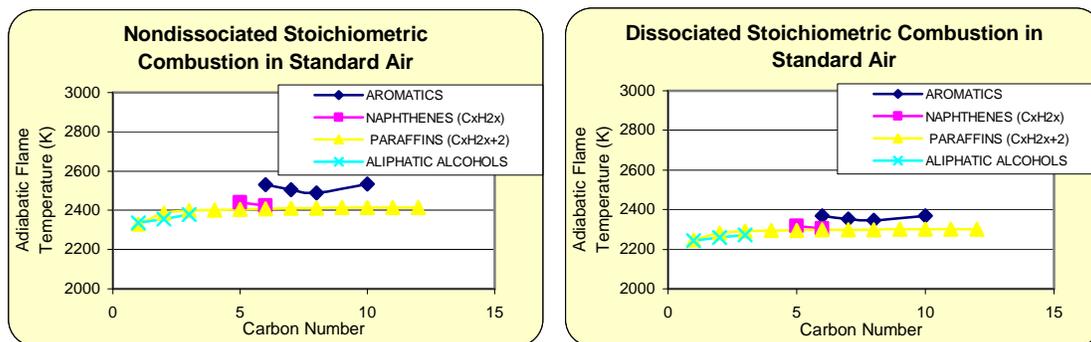


Figure 4. Stoichiometric Adiabatic Flame Temperature as a Function of the Fuel Carbon Number

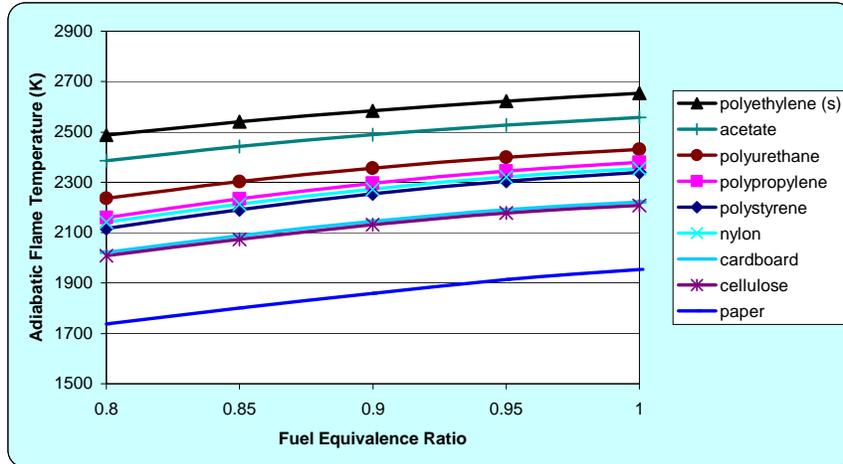


Figure 5. Adiabatic Flame Temperature (K) of Different Plastics and Non-Plastics vs. Equivalence Ratio

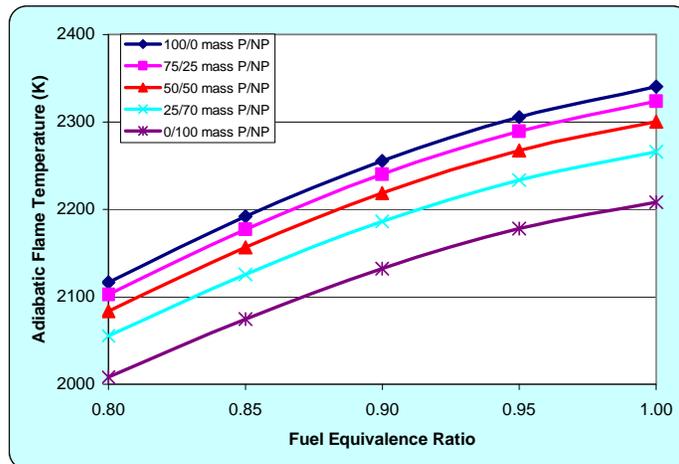


Figure 6. Adiabatic Flame Temperature (K) of Mass Mixtures of Plastics (P) and Non-Plastics (NP) vs. Equivalence Ratio

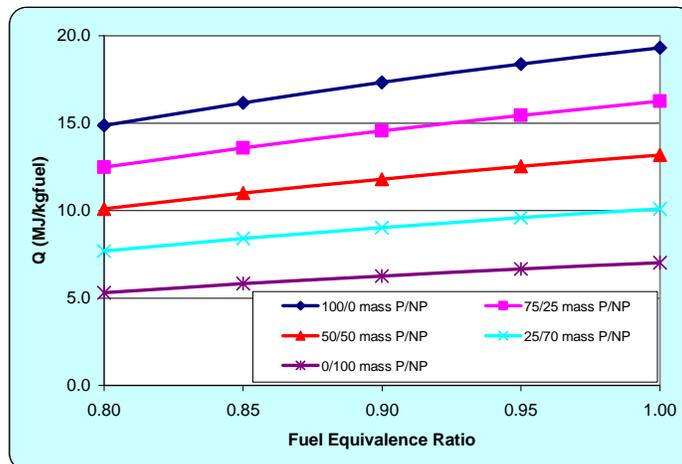


Figure 7. Heat Transfer From Flame at 1500K vs. Equivalence Ratio for Various Mass Mixtures of Plastic/Non-Plastic

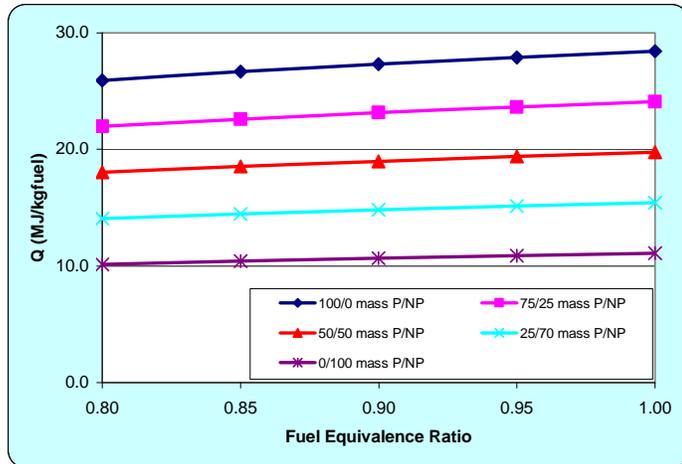


Figure 8. Heat Transfer From Flame at 1000K vs. Equivalence Ratio for Various Mass Mixtures of Plastic/Non-Plastic

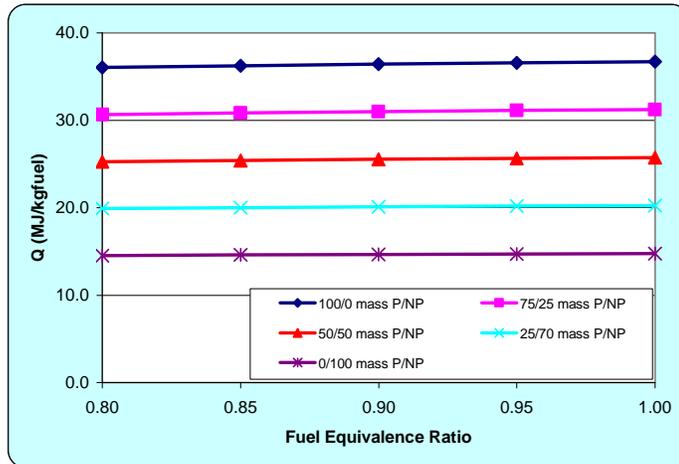


Figure 9. Heat Transfer From Flame at 500K vs. Equivalence Ratio for Various Mass Mixtures of Plastic/Non-Plastic

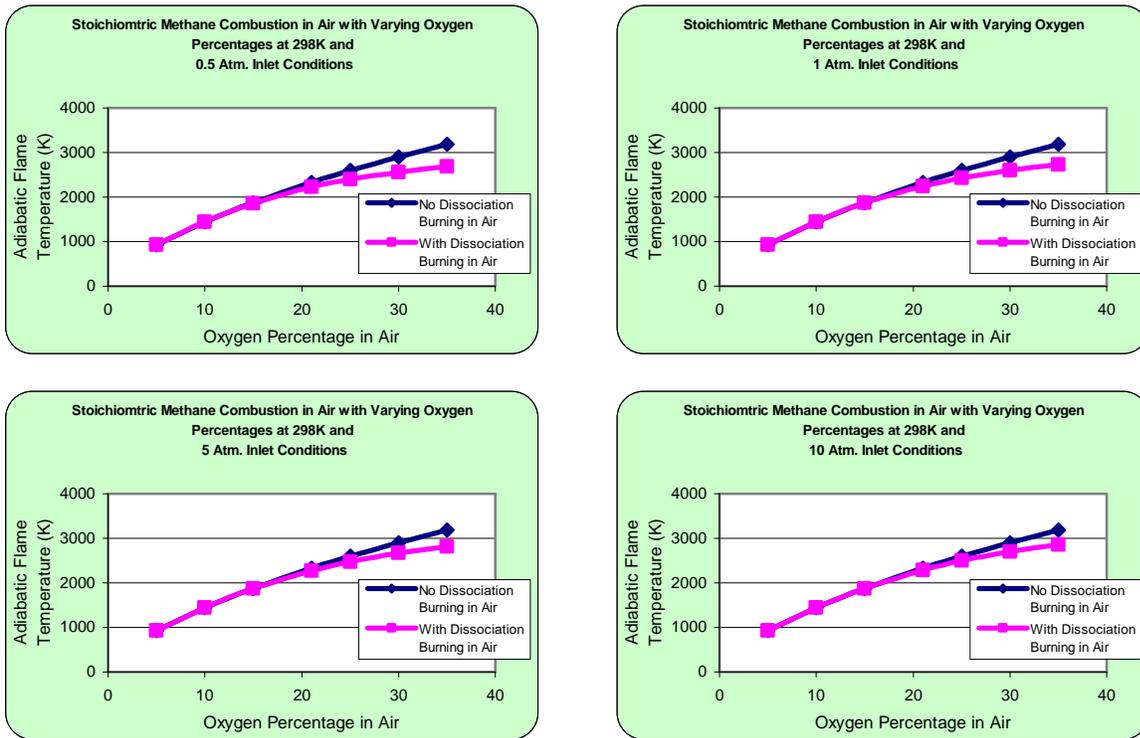


Figure 10. Flame Temperature for Methane Burning in Stoichiometric "Air", as a Function of Oxygen Percentage and for Varying Combustion Pressures

APPENDIX A

ADIABATIC FLAME TEMPERATURE CALCULATION: Computational Methodology for General CHONS Fuels

1. PRODUCT SPECIES

1.1 Chemical Balance

The discussion is restricted to typical hydrocarbon fuels of the form C_xH_y where x and y are known for the fuel of interest. Additionally, oxygen, nitrogen and sulfur may be specified as part of the fuel. The paraffins have $y = 2x + 2$ and include the most familiar fuels: methane CH_4 , propane C_3H_8 , butane C_4H_{10} , and decane $C_{10}H_{22}$. The results will illustrate computations with these four fuels; other fuels can be handled in a similar fashion.

Focusing on 1 kg-mole of fuel, the general expression for burning of a hydrocarbon fuel in air is



The right hand side represents the major combustion product species. Without dissociation the n_i -values are readily specified (so-called "cold" products of combustion), see Section 1.2. With dissociation the n_i -values are deducible via a half-interval search technique at a given temperature, see Section 1.3. With more detailed dissociation consideration, additional right hand side product species occur, including O, H, OH, and NO. Information on handling these extra complexities is also given in Section 1.3.

If burning takes place in oxygen alone, then $f = 0$ and $n_4 = u/2$. If the oxidant is air, then $f = 3.76$ since oxygen represents 21 percent of air by volume and nitrogen is reckoned to provide the other 79 percent. These values are consistent with 23.2 percent oxygen by mass, and 76.8 percent nitrogen by mass. The value of m is determined from the burning conditions (the amount of oxidant supplied relative to the amount of fuel supplied). It controls strongly the amount of product species (the n_1, n_2, \dots, n_7 values, the kg-mole amounts of product species produced from the burning of 1 kg-mole amounts of product species produced from the burning of 1 kg-mole of fuel). Two values of m have special significance in determination the **nondissociated** products produced (the products observed when their temperature is low). These two values are:

1. **Stoichiometric** $m = m_s = x + y/4 - z/2 + v$

This amount of oxidant produces entirely CO_2 and H_2O in the product stream and their amounts are determined. There is no CO or O_2 in the products. The familiar **stoichiometric** (chemically-correct) reaction expression is Eq. (1) with

$$\begin{aligned} m &= m_s \\ n_1 &= n_5 = n_6 = 0 \\ n_2 &= x \\ n_3 &= y/2 \\ n_4 &= mf + u/2 \\ n_7 &= v \end{aligned}$$

2. **Minimum air** $m = m_{\min} = x/2 + y/4 - z/2 + v$

This amount of oxidant is just enough to oxidize all the fuel to CO and H_2O . There is no CO_2 or O_2 in the products. The familiar **minimum oxidant** reaction expression in Eq. (1) with

$$\begin{aligned}
m &= m_{\min} \\
n_2 &= n_5 = n_6 = 0 \\
n_1 &= x \\
n_3 &= y/2 \\
n_4 &= mf + u/2 \\
n_7 &= v
\end{aligned}$$

The chemically-correct m for stoichiometric burning ($m_s = x + y/4 - z/2 + v$) serves to define the **equivalence ratio** \emptyset of a particular reaction with user-specified m via:

$$\emptyset = m_s/m$$

For a given fuel or fuel blend, m and \emptyset are related easily with each other. A general burn is either:

1. Fuel rich $\emptyset > 1$ and $m < m_s$
2. Fuel lean $\emptyset < 1$ and $m > m_s$
3. Stoichiometric $\emptyset = 1$

and the nondissociated products are easily determined from x , y and m of the given problem, as illustrated in Section 1.2. Notice that $n_6 = 0$ in all the nondissociated product cases.

1.2 Product Species Without Dissociation

The hotter the product species are, the more the assumption of nondissociated products will be incorrect, and flame temperatures calculated with this assumption will also be increasingly in error. In the present section, product species are considered without dissociation; in Section 1.3, this restriction is removed and product species amounts with the inclusion of dissociation are calculated.

The values of x , y , z , u , v and m determine the product species molar (volumetric) amounts. If fuel lean $m > m_s$ and there is no CO or H₂ in the products, and, see Borman and Ragland (1998) and Turns (2001), we have

$$\begin{aligned}
n_1 &= 0 \\
n_2 &= x \\
n_3 &= y/2 \\
n_4 &= mf + u/2 \\
n_5 &= m - m_s \\
n_6 &= 0 \\
n_7 &= v
\end{aligned}$$

If fuel rich $m < m_s$ and there is no O₂ or H₂ in the products, it is assumed that the lack of sufficient oxygen affects the CO₂ only (part of the C oxidizing only as far as CO). The very reactive hydrogen H is assumed to fully oxidize to H₂O. Then, again see Borman and Ragland (1998) and Turns (2001), we have

$$\begin{aligned}
n_1 &= 2(m_s - m) \\
n_2 &= 2(m - m_{\min}) \\
n_3 &= y/2 \\
n_4 &= mf + u/2
\end{aligned}$$

$$n_5 = 0$$

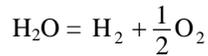
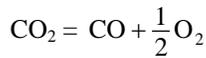
$$n_6 = 0$$

$$n_7 = v$$

These equations hold for $m \geq m_{\min}$ only. The cases $m < m_{\min}$ are of limited interest, for then not all the fuel burns, flame temperatures are low, ignition is a problem, and poor flames result. These extreme fuel-rich flames will be excluded from further discussion.

1.3 Product Species with Dissociation

One of the simplest, effective and most useful assumptions about dissociation is that at high temperatures some of the CO_2 in the product stream will dissociate into CO and O_2 and some of the H_2O in the product stream will dissociate into H_2 and O_2 . This dissociation absorbs energy and reduces the temperature of the product stream. This main dissociation is represented via



The amount of dissociation depends on pressure and temperature, and is such that the molar (volume) fractions obey the laws of mass action. Following Goodger (1977) and Campbell (1979), these can be written in the form

$$K_{\text{CO}_2} = \frac{n_2}{n_1} [n_T / (n_5 p)]^{1/2} \quad (2)$$

$$K_{\text{H}_2\text{O}} = \frac{n_3}{n_6} [n_T / (n_5 p)]^{1/2} \quad (3)$$

where n_1, n_2, \dots, n_7 are the molar species amounts (see Eq. (1)), p is the total pressure (in atmospheres), and $n_T = n_1 + n_2 + \dots + n_7$. The value of the partial pressure equilibrium constants K_{CO_2} and $K_{\text{H}_2\text{O}}$ can be expressed in terms of temperature T via

$$K(T) = \exp [a/T + (b + c/T) \ln T + d] \quad (4)$$

where T is in degrees Kelvin, and the coefficients a, b, c and d are constants given in Table 1 (from Campbell, 1979) for the useful range $1600 < T < 6000$.

Table 1 Coefficients for Eq. (4)

Constant	a	b	c	d
K_{CO_2}	33,805.0	0.7422	165.8	-16.5739
$K_{\text{H}_2\text{O}}$	42,450.0	-1.074	-2,147.0	3.2315

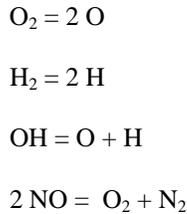
The two equations, Eqs. (2) and (3), are supplemented by five chemical element balance equations from Eq. (1):

$$\begin{aligned}
 n_1 + n_2 &= x \\
 2n_3 + 2n_6 &= y \\
 n_1 + 2n_2 + n_3 + 2n_5 &= 2m + z \\
 n_4 &= mf + u/2 \\
 n_7 &= v
 \end{aligned}$$

These seven equations, at a given pressure and temperature, suffice to determine the product stream coefficients n_1, n_2, \dots, n_7 .

If the temperature of the product stream is known, a half-interval search technique can be used (for the species molar amounts n_i) as described in Goodger (1977). The initial estimate for the molar fraction of oxygen (taken as 0.4 is usually satisfactory) is sequentially refined until the seven n values simultaneously satisfy the required seven equations. A half-interval search technique is used; it is robust and converges rapidly.

After the main dissociations of CO_2 and H_2O are established, further dissociation of the product species can be determined in a similar fashion, via:



with partial pressure equilibrium constants similar to Eqs. (2) and (3), and given by fitted curves like Eq.(4). Parameters for the calculation of the K values are available in a form similar to Table 1.

If the product stream temperature is unknown, an outer loop with half-interval search for temperature is needed – it is described in the next section.

2. TEMPERATURE

2.1 Energy Balance

Consider 1 kg-mole of fuel and other reactants entering and reacting inside a control volume fixed in space. The products of combustion leave the control volume. The process is supposed to be in steady state operation at constant pressure. No work is done by the gaseous mixture in the control volume, but heat is supplied to it in the amount of Q Joules per kg-mole of fuel entering. The appropriate steady flow energy equation version of the first law of thermodynamics (neglecting kinetic energy which is usually small in combustion cases relative to other changes) is simply

$$Q = P - R = \sum n_e h_e - \sum n_i h_i \quad (5)$$

where P = total energy in product stream, R = total energy in reactant stream, and the summations are over all species energies, n_e = kg-moles of species e , and h_e = specific enthalpy of species e in Joules/kg-mole of species e (in exit stream), and n_i and h_i are similarly defined for the inlet stream. The h_e and h_i depend on the species in question and temperature. The fuel stream enthalpy **includes** its chemical enthalpy (the energy it releases when burned), this being calculated in the computer code from its given "**Heating Value**" or "**Heat of Combustion**".

When Q equals zero, the temperature of the product stream is called the **adiabatic flame temperature**. When both reactants and products are at 298 K, the heat added (Q J/kg-mole of fuel – usually Q is negative since typical combustion reactions are exothermic) to achieve this is the negative of the **heat of combustion** of the fuel (J/kg-mole of fuel), quoted as the net (lower) value if the product species are considered to be in gaseous form, and as the gross (higher) value if product species condense to liquid form. Other names are: calorific value, heating value, and enthalpy of combustion (reaction).

2.2 Enthalpy Calculations

Following Campbell (1979), the enthalpies (kJ/kg-mole of species) of the high temperature ($1600 < T < 6000$) gaseous product species may be expressed as

$$h = A + BT + C \ln T \quad (6)$$

with T in degrees Kelvin. Table 2 gives the constants for the six product species of interest.

Table 2. Coefficients for Eq. (6)

Species	A	B	C
CO	309,070.	39.29	-6,201.9
CO ₂	93,048.	68.58	-16,979.0
H ₂ O	154,670.	60.43	-19,212.0
N ₂	44,639.	39.32	-6,753.4
O ₂	127,010.	46.25	-18,798.0
H ₂	461,750.	46.23	-27,649.0

For most hydrocarbon fuels, heating values are typically about 45 MJ/kg of fuel, tables of values are readily available in thermodynamics and combustion texts. For example:

Methane	50.05 MJ/kg	Propane	46.39
Butane	45.77	Decane	44.63

These values are input to the computer code, and then internally calculation is made of the "fuel enthalpy" which is easily calculated using a stoichiometric version of Eq. (5) with reactants and products at 298 K, and nondissociated gaseous species in the product stream.

Table 3. Enthalpies of reactants at 298 K

Species	Enthalpy kJ/kg-mole
CH ₄	887,166.
C ₃ H ₈	2,204,156
C ₄ H ₁₀	2,856,436.
C ₁₀ H ₂₂	6,769,800.
O ₂	17,200.
N ₂	15,780

The so-calculated "enthalpies" of the reactant species are given in Table 3; these values include the chemical enthalpy of the fuel. If the reactants enter at temperatures higher than 298 K, additional enthalpy is calculated using appropriate specific heat values and the temperature range. Note that the fuel enthalpy includes the "chemical enthalpy" of the fuel, so that this amount of total reactant energy is all-important. For the adiabatic flame temperature, one seeks a temperature at which the total enthalpy of the products is equal to this reactant energy. When the product stream temperature is known, a calculation of the heat transferred inside the combustor/furnace is simply calculated as the difference between the energies of the reactants and the products.

2.3 Temperature Calculations

Adiabatic flame temperatures are found using a half-interval search technique, seeking to find a product species temperature for which Q is zero, see Eq. (5). The method is described in Campbell (1979). The first trial for T is 4000 K, and the first ΔT correction is 2000 K. The procedure is:

1. Guess T of products
2. Calculate $Q = P - R$
3. If Q is positive, take new $T = T - \Delta T$
If Q is negative, take new $T = T + \Delta T$
4. Half ΔT
5. Return to step 2

Steps 2 through 5 are repeated until Q is small. Typically, 15 such iterations are used to obtain the outlet temperature to within 1 degree Kelvin.

When used with known nondissociated product species amounts of Section 2.2, the half-interval search for product temperature is the only iterative sequence required. When used with dissociated product species amounts, which depend on temperature, see Section 1.3, the half-interval search for temperature provides an outer loop. An inner loop is for the product species amounts, using another half-interval search described in Section 1.3.

3. THE COMPUTER CODE

3.1 The Computer Code Structure

AFTC is a computer code that has two capabilities. One possibility is calculating the **adiabatic flame temperature** and the product species for the given reactants. The second possibility is that of calculating the **amount of heat transferred** within the combustor when a specified exit stream temperature is given. After the dimension and data segments, the code is divided into eight chapters:

1. Preliminaries and four problem loops
2. Outer loop for product outlet temperature
3. Inner loop for product species amounts
4. No dissociation case, product species are known
5. Dissociation calculations for product species
6. Check sum of product species for convergence
7. Check first law for adiabatic reaction
8. Storage, loop terminators and final print

3.2 Problem Specification/Data Input

The situation considered in the computer code has the following data:

1. Enthalpy and fuel identification characters (x, y, z, u, v)
2. Enthalpy–temperature expression parameters
3. Inlet temperatures of the fuel and oxidant streams
4. In "air" as the oxidant, specification of the percent by volume in the air is permitted
5. Dissociation case: total pressure in atmospheres and partial pressure equilibrium constants of CO₂ and H₂O – these are calculated from fitted curves vs temperature

The above data are input in the data segment. SI units are used exclusively.

3.3 Solution Algorithm

The user specifies the **fuel** via the input table which has a range of fuels already included, and the molar amounts of each fuel component in the case of a composite fuel. Any new fuel can easily be specified via its C, H, O etc content and its lower heat of combustion. Internally, the stoichiometric and minimum air m values are then calculated. The multiplier m of the "air" or oxidant bracket of Eq. (1), with prompts as to the m_s and m_{\min} values for his specified fuel. The user also specifies the **equivalence ratio** from which the air bracket multiplier m is calculated. A further prompt requests the **oxygen volume percent** of the "air" stream, for the air-fuel reaction; from the value supplied, the f -value is calculated. If the default value of 21 percent is taken, a value of $f = 3.76$ results. The user is also prompted to supply **inlet temperatures of the reactant streams** (typically 298 degrees K. The **combustor pressure** is supplied in atmospheres. He is makes the choice for finding the **adiabatic flame temperature** (in which case this is calculated in the code) or specifying the **outlet temperature** (in which case the heat transferred inside the combustor is calculated).

Internally, two nested loops control the solution procedure according to the problem situation. These loops handle the following parameters:

1. Dissociation effect loop – where this effect is to be considered or not
2. Oxidant loop – which determines the burning to be in "air" or oxygen

The VBA code behind the Excel sheet is written and divided into "Chapters". The initial estimate of outlet temperature is given in Chapter 2 of the computer code, taken as 4000 degrees K. Two nested iteration loops are need to converge upon the correct temperature and species amounts.

The **outer loop of iterations** provides a half-interval search for the correct outlet temperature for an adiabatic reaction is used; the first law is checked in Chapter 7 of the computer code, a revised estimate of the temperature is calculated, and control is returned to Chapter 2. This provides the outer loop.

An **inner loop for the product species molar amounts** when dissociation is included; otherwise, no inner loop iterations are needed. With dissociation, an initial estimate of the ratio n_5/n_T is given in Chapter 3 of the computer code. This represents the number of moles in oxygen in the product divided by the total number of moles in the product. A half-interval search for the correction ratio and the product species amounts is used; the check is made in Chapter 6, a revised estimate is calculated, and control is returned to Chapter 3. This provides the inner loop.