GENERALIZED FLAME TEMPERATURE AND

SPECIES CALCULATIONS USING EXCEL/VBA

By

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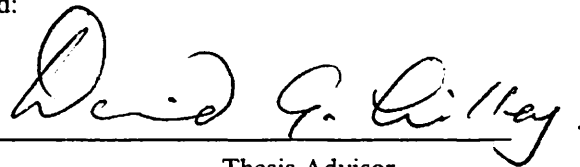
Fort Collins, Colorado

2002

Submitted to the Faculty of the
Graduate College of the
Oklahoma State University
in partial fulfillment of
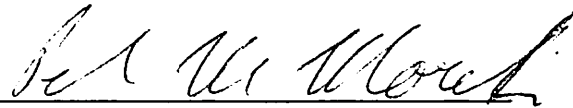the requirement for
the Degree of
MASTER OF SCIENCE
December, 2004

GENERALIZED FLAME TEMPERATURE AND

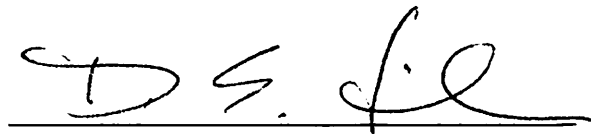# SPECIES CALCULATIONS USING EXCEL/VBA

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ACKNOWLEDGEMENTS

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NOMENCLATURE

G	Gibb's Free Energy
$g_i{}^\circ$	Reference Gibb's Free Energy
H	Enthalpy
h_p	Product Species Enthalpy
h_r	Reactant Species Enthalpy
K	Partial Pressure Chemical Equilibrium Constant
m	Air/Fuel Ratio
m_s	Stoichiometric Air/Fuel Ratio
n_i	Molar Amount of Species i
P_i	Partial Pressure of Species i
P°	Reference Pressure
p	Nondimensionalized Pressure $\dfrac{P}{P^\circ}$
Q	Heat Transfer within the Combustion Zone
R	Gas Constant
S	Entropy
T	Temperature
y_i	Mole Fraction of Species i
ϕ	Equivalence Ratio $\dfrac{m_s}{m}$

CHAPTER ONE

Introduction

1.1 The Problem

It is often necessary to know the maximum flame temperature and corresponding product composition in a chemically reacting system. However, experimentation to find combustion temperatures and product species is extremely delicate, costly, and time consuming. For this reason, theoretical methods are preferred, where a model can be checked against a limited set of experimental data. 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 nondissociated 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.

The adiabatic flame temperature, theoretically the maximum temperature reached, depends mainly on: the type of fuel and oxidizer and their respective amounts, the

reactant inlet temperatures, the amount of oxygen in the air, dissociation effects, and the level of dissociation assumptions used.

1.2 Previous Studies

The material presented in Van Wylen and Sonntag (1985) is typical of that studied in standard undergraduate thermodynamics courses. Textbooks present the ideas of chemical reactions, dissociation, flame temperature, and product species, but the techniques are often given in a manner that is not computerizable. Often, even the computerized methods given lack generality.

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 Kretchmer (1986), and combustion aerodynamics and its applications, see Beer and Chigier (1972) and Gupta and Lilley (1985). Again, none of these texts give general computerized methods for finding the adiabatic flame temperature and product species amounts. 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 computerized calculations of flame temperature (Borman and Ragland (1998) and Turns (2001)) with the inclusion of computer codes, see Turns (2001).

1.3 Objectives of the Present Study

Using the methods of Goodger (1977) and Campbell (1979), a straightforward computer code is 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. 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 (2004). Results are given for a range of input parameters and displayed in Appendices A and B.

CHAPTER TWO

Theoretical Background

2.1 Chemistry

Combustion, i.e. the act of burning a fuel in an oxidizer, is simply a chemical reaction in which the reactants, the fuel and the oxidizer, become the combustion products through an exothermic chemical reaction. The traditional way to express this in chemical notation is:

$$aA + bB \Rightarrow cC + dD \tag{1}$$
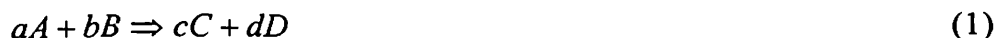
where the left hand side of the equation consists of the reactants and the right hand side contains the products. The capital letters denote the individual species, and the lower-case letters denote the number of moles of each respective species. If exactly the right quantity of oxidizer is supplied to the reaction to fully oxidize the fuel, the reaction is "stoichiometric." If there is not enough oxidizer, the reaction is "fuel rich." Likewise, if there is too much oxidizer, the reaction is "fuel lean." Furthermore, if the products are limited to those that result from completely oxidizing the reactants' atoms, combustion is considered "complete." Complete combustion is an approximation; however, because real combustion is inhibited by Second Law effects, leading to the dissociation of the component molecules. Dissociation will be discussed later in this paper. Incomplete combustion also occurs if there is not enough oxygen to complete all the oxidation reactions necessary. The only time complete combustion could be attained without ignoring the Second Law is if the reaction temperature stays well below 1000K. Roy

(2002). Such combustion is termed "cold combustion." By definition, fuel rich combustion cannot be complete.

For example, if methane burns in oxygen as per:

$$CH_4 + 2O_2 \Rightarrow 2H_2O + CO_2$$

it would be classified as complete stoichiometric combustion. However, if extra oxidizer were added and additional molecules were allowed in the products as per:

$$CH_4 + 3O_2 \Rightarrow n_{CO}CO + n_{CO_2}CO_2 + n_{H_2O}H_2O + n_{O_2}O_2 + n_{H_2}H_2$$
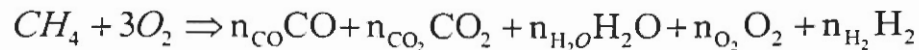
it would be classified as fuel lean combustion. Note the number of moles of each product species cannot be directly computed from atom balances. These values can be calculated by using chemical equilibrium equations, which are discussed later in this paper.

2.2 Air as Oxidizer

At this point, a note must be made about air. Air is the most common oxidizer used in combustion for obvious reasons; it is free and readily available for most applications, Wark (1988). The chemical composition varies with location and normal weather phenomenon, but consists primarily of nitrogen and then oxygen. Water vapor, carbon dioxide and trace elements of other species are also typically present. However, for "dry standard air" formulations, air is assumed to consist of only oxygen and nitrogen. Any inert elements are treated as nitrogen and the other trace substances are disregarded. On a volumetric, and therefore molar, basis, standard dry air is composed of 21% oxygen and 79% nitrogen, Wark (1988). Therefore, ((1-.21) / .21 =) 3.762 moles of nitrogen will be included with each mole of oxygen involved in the oxidation process. So, complete stoichiometric methane combustion in dry standard air takes the form of:

$$CH_4 + 2(O_2 + 3.762N_2) \Rightarrow 2H_2O + CO_2 + 2*3.762N_2$$
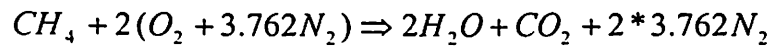
2.3 Assumptions

Several assumptions are made in order to simplify the prediction of the adiabatic flame temperature. First, given the relatively low densities, the common assumption of an ideal gas is used. Also, equilibrium and global reactions are used.

2.3.1 Equilibrium Conditions

A system is in equilibrium when no changes occur within it unless it is affected by its surroundings. This can be further specified. A system is in mechanical equilibrium if the pressure does not change and is in thermal equilibrium if the temperature does not change. Finally, a system is in chemical equilibrium if no changes in the overall chemical composition occur with time, Cengel and Boles (1998). Furthermore, a system in chemical equilibrium is also in thermodynamic equilibrium, Campbell (1979).

The justification for assuming chemical equilibrium is that the chemical reaction forming the products takes place nearly instantaneously, relative to most time scales encountered in engineering practice, Zel'dovich and Raizer (2002). Thus, no time scale need be included in the relations. As no ability for phase changes have been included, phase equilibrium has also been assumed. These equilibrium restrictions are not to say that the components cannot change pressure, temperature, chemical composition, or phase during the reaction, but that they will not change once established on either side of it. For example, hydrogen and oxygen gas, once calculated into the products, will not

combine into water vapor and then condense to liquid form. One result of this is that all the water vapor in the products is assumed to remain in the gaseous state

2.3.2 Global Reactions

The concept of global reactions is also used. Actual chemical reactions are a sequence of intermediate steps, in which molecules are created and destroyed in a series of elementary reactions. The examples listed above are global reactions, Glassman (1987). Turns (2001) lists a complex combustion mechanism for methane. It involves 277 elementary reactions and 49 species. Many reactions involve many times more elementary reactions, Hucknall (1985). So, for the reasons of speed, simplicity, and ease of implementation, global reactions are used. This is justified because these combustion mechanisms are largely limited by a relatively small number of elementary reactions. Furthermore, these reactions only become significant if chemical kinetics are used, Ferguson and Kirkpatrick (2001).

2.4 Dissociation

Previous to this point, only limited dissociation has been described. Dissociation is the act of the molecules splitting apart into simpler molecules and their respective atoms. It occurs most in high temperature and / or low pressure regions. This happens because, as the internal rotational energy increases, the increased centrifugal force within the molecule stretches the atoms apart, Sonntag and Van Wylen (1985).

In terms of analysis, dissociation increases the difficulty of calculating the adiabatic flame temperature and product composition because it adds additional unknowns without, at least at first, additional equations relating these unknowns. This

problem is overcome by using the Gibb's free energy and assuming chemical equilibrium.

Following the methods outlined in Sonntag and Van Wylen (1985), first, consider the general case given from equation one, which will then be restricted to a dissociation reaction, for example,

$$CO_2 \Leftrightarrow \frac{1}{2}O_2 + CO$$
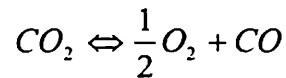
From the Second Law, it is known that the reaction occurs at the maximum entropy because entropy will always increase or remain the same. When the maximum entropy is reached, the product composition is frozen. Likewise, when the Gibb's free energy is minimized, the product composition is frozen, where the free energy is, in terms of enthalpy (H), temperature (T), and entropy (S):

$$G = H - TS$$

Gibb's free energy is used instead of entropy because it contains terms that include readily available species components for the pressure, temperature, and species. The dissociated products are found by minimizing the free energy. Therefore, at equilibrium, for constant temperature and pressure during the reaction, dG = 0, and:

$$\sum_i \overline{G}_i dn_i = 0 \tag{2}$$

where $\overline{G}$ is the molar Gibb's free energy and n is the molar amount of each species. Now, because chemical equilibrium was assumed, there is a relation between the components.

From gas kinetic theory for an ideal gas, in terms of partial pressure (P_i), reference pressure ($P°$), the gas constant (R), and reference Gibb's free energy ($g_i°$), the Gibb's free energy for one species (i) is:

$$G_i = g_i° + RT \ln\left(\frac{P_i}{P°}\right)$$

Or, in terms of mole fractions (y) and a nondimensionalized pressure (p):

$$G_i = g_i° + RT \ln(y_i p)$$

Therefore, after following the convention that $dG = \Delta G$ and substituting back into equation two,

$$\Delta G = \Delta G° + RT \ln\left[\frac{y_C^c y_D^d}{y_A^a y_B^b}(p)^{C+D-A-B}\right]$$

For convenience, the term in the natural logarithm is set to the constant K. Therefore,

$$\Delta G = \Delta G° + RT \ln[K]$$

As a result, at equilibrium, K, now known as the partial pressure chemical equilibrium constant, takes the form:

$$\ln(K) = \frac{-\Delta G°}{RT}$$

Where $\Delta G° = ag°_A + bg°_D + ag°_A + bg°_B$

Returning to the example of the dissociation of carbon dioxide at equilibrium:

for $CO_2 \Leftrightarrow \frac{1}{2}O_2 + CO$, $\ln(K_{CO_2}) = \frac{-\Delta G°_{CO_2}}{RT}$

where $\Delta G°_{CO_2} = \left(\frac{1}{2}\right)g°_{O_2} + (1)g°_{CO} - (1)g°_{CO_2}$

And, from the definition of K,

$$K = \left[\frac{y_{O_2}^{\frac{1}{2}} y_{CO}^{1}}{y_{CO_2}^{1}} (p)^{\nu_2^{'}+1-1} \right]$$

So, if one knows the reference free energies, one has an equation describing the relation between the reactants and the different products.

2.5 Energy Balance

Given the constraints and equations above, the flame temperature can be calculated by enforcing energy conservation from the reactants to the products. Assuming no work is done on or by the system and there are no changes in kinetic or potential energy, from the First Law of thermodynamics, the constant pressure ideal gas energy equation is:

$$Q = P - R \equiv \sum n_p h_p - \sum n_r h_r \qquad (3)$$

where Q is the heat transfer in the combustion zone. For an adiabatic flame temperature calculation, $Q = 0$. P is the total energy of the product stream, and R is the total energy of the reactants. h_p and h_r represent the enthalpies of each species in the products and reactants, on a molar basis. The n coefficient then, is the number of moles of each species. Assuming the enthalpies are functions of temperature only, the temperature that satisfies equation three is the temperature of the chemical reaction. In other words, it is the flame temperature. Enthalpy values are supplied in the JANAF Thermochemical Tables, JANAF (1985) and other, similar references.

CHAPTER THREE

Solution Method

3.1 The Combustion Equation Set

The general chemical expression for burning a CHONS fuel in some oxidizer is:

$$C_xH_yO_zN_uS_v + m\,(O_2 + f\,N_2) \Rightarrow$$
$$n_{CO}CO + n_{CO_2}CO_2 + n_{H_2O}H_2O + n_{N_2}N_2 + n_{O_2}O_2 + n_{H_2}H_2 + n_{SO_2}SO_2$$
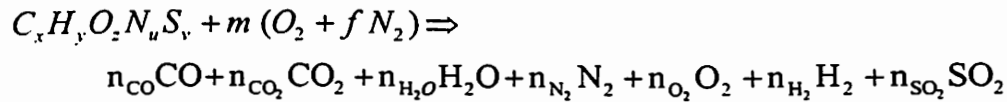
where the right hand side represents the major combustion product species. Without dissociation, the n_i-values are readily determined from atom balances. With dissociation, the extra n_i-values are found via a half-interval search technique at a guessed temperature. Remember, if the oxidant is dry standard air, then $f = 3.762$. The value of am is determined from the given equivalence ratio, ϕ, which is defined as:

$$\phi = \frac{m_s}{m}$$

where m_s is the stoichiometric air / fuel ratio and am is the ratio for the given oxidizer, Ferguson and Kirkpatrick (2001). From atom balances, for a CHONS fuel, one finds the stoichiometric air / fuel ratio is:

$$m_s = x + \tfrac{y}{4} - \tfrac{z}{2} + v$$

The number of moles of each species in the product stream must be calculated in order to apply an energy balance on the reactants and products. For the general case given above, there are seven unknown species. Five can be accounted for through atom balancing:

$$C: \qquad x = n_{CO} + n_{CO_2}$$

H_2: $\qquad \frac{y}{2} = n_{H_2O} + n_{H_2}$

O_2: $\qquad \frac{z}{2} + m = \frac{1}{2}n_{CO} + n_{CO_2} + \frac{1}{2}n_{H_2O} + n_{O_2} + n_{SO_2}$

N_2: $\qquad \frac{w}{2} + m * f = n_{N_2}$

S: $\qquad v = n_{SO_2}$

As mentioned before, the additional species can be attained by using chemical equilibrium constants to describe dissociation reactions. 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. This dissociation absorbs energy and reduces the temperature of the product stream. These two reactions and their respective equilibrium constants are:

$$\frac{1}{2}O_2 + CO \Leftrightarrow CO_2 \qquad\qquad K_{CO_2} = \frac{y_{CO_2}}{y_{CO}y_{O_2}^{1/2}}(p)^{-1/2}$$

$$H_2 + \frac{1}{2}O_2 \Leftrightarrow H_2O \qquad\qquad K_{H_2O} = \frac{y_{H_2O}}{y_{H_2}y_{O_2}^{1/2}}(p)^{-1/2}$$

where y_i are the mole fractions of each species and p is the number of atm. The solution method used to combine these equations is covered in section three.

3.2 Solution for Individual Product Species

AFTC is a computer code that has two capabilities. One possibility is calculating the adiabatic flame temperature and the product species given the parameters as stated in Section 1.3. The second possibility is that of calculating the amount of heat transferred within the combustor when a specified exit stream temperature is given. Regardless,

AFTC finds the combustion temperature and products by applying the methods of Goodger (1977) and Campbell (1979) to the equations outlined in above. Additionally, AFTC finds these values for four different situations: burning in the defined oxidizer or in pure oxygen; and ignoring and including dissociation. Following Goodger (1977) and Campbell (1979), the preceding equations are combined to find the product composition.

$$n_{N_2} = \frac{u}{2} + m * f$$

$$n_{SO_2} = v$$

from which the number of moles of nitrogen and sulfur dioxide in the products are found. Then, rearrange the dissociation reactions in terms of the nondimensionalized pressures:

$$\frac{n_{CO_2}}{n_{CO}} = K_{CO_2} y_{O_2}^{\frac{1}{2}} p^{\frac{1}{2}}$$

$$\frac{n_{H_2O}}{n_{H_2}} = K_{H_2O} y_{O_2}^{\frac{1}{2}} p^{\frac{1}{2}}$$

To use in the following:

$$n_{CO} = \frac{x}{1 + \frac{n_{CO_2}}{n_{CO}}}$$

$$n_{CO_2} = x - n_{CO}$$

$$n_{H_2} = \frac{\frac{y}{2}}{2\left(\frac{n_{H_2O}}{n_{H_2}} + 1\right)}$$

$$n_{H_2O} = \frac{y}{2} - n_{H_2}$$

from which mole numbers for carbon monoxide, carbon dioxide, hydrogen, and water are found.

3.3 The Computer Algorithm

In summary, the computer algorithm for the adiabatic flame temperature is:

```
┌─────────────┐     ┌──────────────┐     ┌──────────────┐     ┌──────────────────┐
│ Initialize  │────▶│  Read Fuel   │────▶│     Read     │────▶│   Calculate      │
│ Variables   │     │  Properties  │     │   Oxidizer   │     │ Molecular Weight,│
└─────────────┘     └──────────────┘     │  Properties  │     │  Air/Fuel Ratio, │
                                         └──────────────┘     │  Fuel Enthalpy   │
                                                              └──────────────────┘

┌──────────────┐     ┌──────────────┐                    ┌──────────────────┐
│ Begin Product│────▶│ Guess Flame  │                    │  Guess Oxygen    │
│Species Loops │     │ Temperature  │                    │  Mole Fraction   │
└──────────────┘     └──────────────┘                    └──────────────────┘

                           Ignore Dissociation ?
                    Yes ◀─────────◆─────────▶ No

              Is the Air/Fuel Ratio Fuel Rich ?
         No ◀──────────◆──────────▶ Yes

   Calc. Fuel Lean          Calc. Fuel Rich
   Product Mole #s          Product Mole #s

                    Find Equilibrium Constant Eqns.

                    Calc. Product Mole Fractions

                         Does SUM1 = SUM2 ?  ──▶ No

                    Calculate Enthalpies

   Return ◀── True

                    Calc. Check 1st Law: Q = P - R

   Q > 0 Decrease Temp Guess      False

   Q < 0 Increase Temp Guess  ──▶ Now have A.F.T. Print Results ──▶ End
   True
```


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3.4 Computerization

3.4.1 Gas Curve Fits

To facilitate computerization, several steps were taken. First, curve fits are used in lieu of tabulated thermodynamic quantities. This saves requiring large blocks of thermodynamic data that would then require an interpolation step. Curve fits for several gases are given in a variety of books. Following the previously outlined method, the curve fits from Goodger (1977) and Campbell (1979) are used. The thermodynamic tables are divided into high temperature (1600K- 6000K) and low temperature (400K - 1600K) ranges, and an enthalpy curve fit in the form:

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

is provided, where A, B, and C are constants characteristic of the chemical species being modeled. The enthalpy, h, has units of kJ/kmol. These values are given in the following table.

Species	A	B	C
CO (400K-1600K)	299,180	37.85	-4,571.9
CO (1600K-6000K)	309,070	39.29	-6,201.9
CO_2 (400K-1600K)	56,835	66.27	-11,634.0
CO_2 (1600K-6000K)	93,048	68.58	-16,979.0
H_2O (400K-1600K)	88,923	49.36	-7,940.8
H_2O (1600K-6000K)	154,670	60.43	-19,212.0
N_2 (400K-1600K)	31,317	37.46	-4,559.3
N_2 (1600K-6000K)	44,639	39.32	-6,753.4
O_2 (400K-1600K)	43,388	42.27	-6,635.4
O_2 (1600K-6000K)	127,010	46.25	-18,798.0
H_2 (400K-1600K)	326,490	40.35	-8,085.2
H_2 (1600K-6000K)	461,750	46.23	-27,649.0

An equilibrium constant curve fit is also given:

$$K = \exp\left[\frac{a}{T} + \left(b + \frac{c}{T} \right) \ln(T) + d \right]$$

where K is the partial pressure chemical equilibrium constant as defined previously. T denotes the temperature, in Kelvin, and the lower case letters are reaction specific curve fit constants. These values are from Campbell (1979).

Constant	a	b	c	d
K_{CO_2}	33,805.0	0.7422	165.8	−16.5739
K_{H_2O}	42,450.0	−1.074	−2,147.0	3.2515

These curve fits were used when possible; however, no sulfur dioxide curve fit was supplied. One was made into the form already employed using thermochemical tables, JANAF (1986). See Appendix C for details. The calculated values of A, B, and C for low and high temperature sulfur dioxide are:

Species	A	B	C
SO_2 (400K-1600K)	37548	62.38	-7953.4
SO_2 (1600K-6000K)	65565	63.45	-11897

Where again, the enthalpy equation is $h = A + BT + C \ln(T)$.

3.4.2 Fuel Enthalpy

The fuel enthalpy calculation is more complicated. Given stoichiometric complete combustion of one mole of fuel, some amount of heat is released. If the products of this reaction are returned to the original thermodynamic conditions, the heat released is known as the heating value (energy per mass of the fuel). There are two forms of the heating value, the higher and lower. The lower heating value assumes all the water in the products is in gaseous form. The higher heating value assumes all the water in the products is in liquid form. Its energy is higher because no energy has been consumed in changing the phase of the water. An energy balance of this is:

$$(h_{fuel} + m_s \cdot h_{O_2} + m_s \cdot f \cdot h_{N_2})_{T_R} = (n_{H_2O}h_{H_2O} + n_{CO_2}h_{CO_2} + n_{N_2}h_{N_2})_{T_R} + LHV_{fuel} \cdot MW_{fuel}$$

All these values are known or can be calculated except for the h_{fuel} term. After rearranging the above equation, the fuel enthalpy, on a molar basis is:

$$h_{fuel} = LHV_{fuel} \cdot MW_{fuel} + (n_{H_2O}h_{H_2O} + n_{CO_2}h_{CO_2} + n_{N_2}h_{N_2} - (m_s \cdot h_{O_2} + m_s \cdot f \cdot h_{N_2}))_{T_R}$$

For reference, typical lower heating values of hydrocarbon fuels are about 45MJ/kg of fuel. For more details on finding the LHV, see Appendix D.

3.5 Program Variations

Two variations of AFTC have also been written. The first, AFTC-composite, allows the user to input an array of up to two hundred fuels. The fuels are merged into one fuel for the flame temperature calculations. The user chooses composition of the composite fuel by setting the mole fraction of each component fuel. 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 program is also nested in multiple loops. The interior loop runs the basic AFTC code seven times, each time changing the oxygen percentage of the air as per the user's input. Likewise, the outer loop then runs each of these inner loops over a series of seven reactant temperatures. In this way, forty-nine sets of data for a given pressure and equivalence ratio may be generated quickly and easily. Furthermore, the iterated steps are displayed on succeeding pages within the spreadsheet, with each page showing convergence for each case.

The other variation of AFTC, 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. While the temperature and products are

calculated for each fuel in turn, only one set of data is displayed for manageability. This allows fast generation of graphs and tables that may be used to compare different fuels and properties, such as how the adiabatic flame temperature varies with the carbon number of a fuel.

CHAPTER FOUR

RESULTS

A referenced fuel listing with each fuel's CHONS formula and Lower Heating Value can be found in Appendix E.

4.1 General Results for Hydrocarbon Fuels

As the first example of the application of AFTC, four hydrocarbon fuels have been considered: methane (CH_4), propane (C_3H_8), butane (C_4H_{10}), and decane ($C_{10}H_{22}$). Extended results with several different equivalence ratios have been used for each fuel burning in air and pure oxygen. Both dissociation and no dissociation cases are considered. Theses results are shown in Figures 1 through 4, and show trends very close to values expected from data in other calculation procedures given in textbooks. Peak temperatures occur at or near the stoichiometric equivalence ratio. In all cases, burning in pure oxygen yields much higher temperatures than in standard air, and including dissociation forces these values down.

With each case of adiabatic flame temperature, there is a corresponding list of product mole fractions: CO, CO_2, H_2O, N_2, O_2 and H_2. For nondissociated reactions, the species amounts can be found through atom balancing, as in Section 3.1. With dissociation, a half interval search for the oxygen mole fraction must be performed, as outlined in Section 3.3.

4.2 General Oxidizer and Inlet Temperature Effects

4.2.1 Stoichiometric Oxygen-Fuel Flames

Results for the higher temperature stoichiometric oxygen-fuel flames are given in Table 1. Notice that the effect of dissociation is quite dramatic, typically lowering the temperatures by about 2000 K, from 5000+ to 3000+ degrees K. Also, the amount of dissociation of CO_2 and H_2O is dramatic, especially with the CO_2, which is more prone to dissociate, since its equilibrium constant values are considerably smaller than those of H_2O.

Figure 5 plots the results of Table 1, for methane, propane, butane, and decane, burning in pure oxygen. Note the dramatic effect of dissociation on the temperature reduction and species composition for each of the four fuel figures. It is also immediately evident from the graphs that the flame temperatures and product compositions are very similar, irrespective of the fuel used. This means dissociation affects them all, and at such high temperatures, the combustion can hardly be considered "complete."

4.2.2 Stoichiometric Air-Fuel Flames

Results for the lower temperature stoichiometric air-fuel flames are given in Table 2. Standard air with 21% oxygen by volume is being used as the oxidizer. Molar fractions (equal to volume fractions) are also given. Compared with Table 1, the temperatures are significantly lower, consistent with the additional thermal ballast of nitrogen taking part of the heat released, and thereby lowering the combustion product temperature. Dissociation effects are rather minimal, typically lowering the temperatures by about 100 K, from 2300+ to 2200+ degrees K. Hence, this justifies the traditional

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approach in elementary thermodynamics of taking the amounts of product species as if they were "cold" products of combustion. The dissociation effect with fuel-air combustion is even less noticeable for non-stoichiometric conditions, in which even lower temperatures occur. No figures are needed for illustration.

4.2.3 Methane Flames with Various Fractions of Oxygen in the "Air" with Standard Inlet
Temperatures

In Table 3, adiabatic flame temperatures are given for methane fuel flames only, but this time the volume percent oxygen in the "air" is varied, the rest of the "air" being nitrogen. Inlet fuel and oxidant streams both enter at 298K. Results for the range of oxygen-deficient to oxygen-enriched "air" are shown, that is with 10, 15, 21 (standard air), 25 and 30 percent oxygen in the "air". The effects are dramatic, and show the expected trends of the effect of the amount of excess thermal ballast of nitrogen. Less nitrogen is there with stoichiometric combustion when the oxygen volume percent is increased to 30 percent than with lower oxygen percentages. Hence, flame temperatures are higher as the percent oxygen increases in the "air" while still keeping stoichiometric conditions. At these higher temperatures, the dissociation effect is more pronounced, dropping about 300 degrees K from about 2900 K to 2600 K for the 30 percent oxygen case. By contrast, the 10 percent oxygen "air" case has a calculated flame temperature just over 1400 K and no dissociation effect whatever. But, of course, the equations used know nothing of the reality that supporting flames with this low amount of oxygen concentration is generally not possible, except with judicious amounts of pre-heating of the fuel and "air" inlet streams, resulting in higher temperatures and greater propensity for combustion propagation. These concepts are used in the very important, new, and

novel topic of high temperature air combustion, with very wide-ranging applications, Tsuji (2003).

Figure 6 illustrates the effect of the oxygen volume percentage, and the results given in Table 3. Below standard 21% oxygen, there is very little difference between the dissociated and non-dissociated results. It is not until the "air" is enriched to about 25% oxygen that the dissociated products are in the 1% volume fraction range. CO and O2 reaches 3.5% and 2.5% respectively of the product stream when the "air" is 30% oxygen. Together, these dissociated results will impact any product stream analysis. Again, this illustrates the influence nitrogen has on high temperature chemical reactions.

4.2.4 Methane Flames with Various Fractions of Oxygen in the "Air" with Elevated Inlet
     Temperatures

Table 4 and Figure 7 repeat the calculations of Table 3 and Figure 6, but with the inlet fuel and oxidizer inlet temperatures both increased to 1000K instead of the standard 298K. Clearly, this 702K increase does not fully show itself in the final flame temperature because of the higher specific heats at the higher temperatures. The combustion pressure has been kept at 1 atm. As expected, the flame temperatures are higher than those at the lower inlet temperatures in Table 3 and Figure 6; about 500K for no dissociation, and an average of 370K with dissociation. Interestingly, this temperature difference decreases as oxygen percentage in the "air" increases. This can be explained by greater dissociation effects at the higher flame temperatures. Notice that higher inlet temperatures increase dissociation over lower inlet temperatures (see Tables 3 and 4). However, the higher inlet temperature cases can produce similar amounts of dissociation

by reducing the oxygen percentage in the "air" stream. These trends are also important in high temperature combustion, where the effects of dissociation are more severe, and occur in even oxygen-depleted environments.

4.2.5 Methane Flames with Various Fractions of Oxygen in the "Air" with Elevated Inlet

Temperatures at Different Equivalence Ratios

Figures 8, 9, and 10 expand upon the previous sections by illustrating the combined effects of increasing the inlet temperature while varying the oxidizer composition for several different equivalence ratios. Figure 8 gives the basic case of stoichiometric combustion for the various changes listed above. Again, note increasing the inlet temperatures and oxygen percentages does not result in a linear increase in the adiabatic flame temperature. This is particularly true for dissociated combustion. Figure 9 repeats the calculation for 20% fuel lean conditions. Across the curve, the flame temperatures are reduced due to the lack of fuel in the reaction. Concurrently, dissociation is also reduced at all points on the curve. Likewise, Figure 10 shows a corresponding decrease in flame temperatures when there is not enough air to fully oxidize the fuel. As with fuel lean combustion, the degree of dissociation drops as the "air" is depleted of its oxygen.

4.2.6 Methane Flames with Various Fractions of Oxygen in the "Air" at Different

Combustion Pressures

Figure 11 demonstrates the chemical reaction's dependency on the combustor pressure with two flame temperature curves, one for dissociation and one for no dissociation. The first graph has a low pressure of half an atm. and serves to illustrate the

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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 in Figure 11 by noting 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.

4.3 Application of AFTC to High Temperature Air Combustion

A common method used to dispose of municipal solid waste (MSW) is to simply burn it. However, to meet environmental regulations, these incinerators must operate in a way that minimizes pollution. This is accomplished through high temperature air combustion, in which the reactants are raised to some temperature before burning. Under normal conditions, this would increase the dissociated products (pollution) except the oxidizer is oxygen-depleted air. Thus, the temperature rise is minimized.

4.3.1 Methane Flames Burning in Oxygen-Deficient "Air" at Different Equivalence Ratios, at Three Different Inlet Temperatures

In Figure 12, a series of three graphs is given, one each for inlet temperatures of 298K, 1000K and 1500K. The adiabatic flame temperature is plotted against the equivalence ratio for a variety of oxygen percentages of the "air." Note that (in all three inlet temperature cases) as the oxygen percentage increases in the "air", the flame temperature increases, because of less nitrogen with the "air". This is with any one value of the equivalence ratios. Note also that, as the oxygen percentage in the "air" increases, the slope of the adiabatic flame temperature versus equivalence ratio curve steepens,

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demonstrating the temperature dependence on the equivalence ratio. But, notice that at the very lowest oxygen percentages, the temperature versus equivalence ratio curve is nearly flat. This trend occurs regardless of the initial fuel and "air" temperature. Since pollution control requires low oxygen percentages, the remainder of the results will use stoichiometric conditions to present several trends in high temperature air combustion.

4.3.2 Methane Flames with Oxygen-Deficient "Air" with Standard Inlet Temperatures

In Table 5, adiabatic flame temperatures are given for methane fuel flames only, but the volume percent oxygen in the "air" is varied, with the rest of the "air" being nitrogen. Inlet fuel and oxidant streams both enter at 298K. Trials cover a range of oxygen-deficient "air": 2.5%, 5.0%, 7.5%, 10%, 12.5%, and 15%. The standard value of 21% oxygen is included for comparison. The effects are dramatic, and show the expected impact of the excess nitrogen driving down the flame temperatures. At 5% oxygen by volume, the program shows the flame temperature to be less than 1000K. At such low temperatures, dissociation is negligible. In fact, noticeable amounts of dissociated products do not appear until the "air" is made up of greater than 15% oxygen. In these conditions, carbon monoxide production is kept low.

Figure 13 illustrates the effect of the oxygen volume percentage, and the results given in Table 5. Below 15% oxygen, there is no difference between the dissociated and non-dissociated results. Even at 15% levels, the portion of dissociated products is small, and is having little effect on the adiabatic flame temperature. Of course, a municipal incinerator would still require pollution controls, but its operating temperature would not have been affected very much.

4.3.3 Methane Flames with Oxygen-Deficient "Air" with Elevated Inlet Temperatures

Section 4.3.2 demonstrates the extra nitrogen in the oxidizer suppressing pollution with these lower combustion temperatures. However, flame temperatures need to be in excess of 1123K in order to burn organic compounds; Meraz, et al (2003). By Table 5, this will not occur until about 7.5 percent oxygen. However, it is desirable to minimize the oxygen content in the "air" as much as possible. This is accomplished by raising the initial temperatures of the fuel and "air". Tables 6, 7 and 8 repeat the calculations given in Section 4.3.2, but now for inlet temperatures of 1000K, 1250K and 1500K respectively. The essence of these results is also shown in graphical form in Figures 14 and 15, for the cases of inlet temperatures of 1000K and 1500K, respectively.

As one can see in Table 6, by increasing the inlet conditions to 1000K, the adiabatic flame temperature rises above 1200K, at just 2.5% oxygen. This exceeds the 1123K requirement listed above by a narrow margin. At higher inlet temperatures still, the flame temperature will comfortably beat 1100K. For example, at 1500K starting conditions, the corresponding adiabatic flame temperature increases to 1680K. While peak-operating efficiency may be at some other set of parameters, these figures show several interesting trends. Like at lower temperatures, because of the preponderance of nitrogen, the effect of dissociation on the flame temperature is minimal. Furthermore, with so little oxygen available, even at such high temperatures, there is very little generation of pollutants.

4.3.4 Summary of the General Results for Stoichiometric Methane Flames Burning with

Oxygen-Deficient "Air" and Elevated Inlet Temperatures

To summarize the parameter effects, general concepts, and ideas about the trends found are now discussed. The flame temperature produced depends strongly upon the oxygen fraction in the incoming "air", and the initial temperature.

Figure 16 portrays the temperature rise of the product stream; that is, it gives the difference of the product temperature and the inlet temperature. It compares it to the oxygen volumetric percent of the "air" for 500K, 1000K, and 1500K inlet temperatures. Notice that, as the oxygen fraction in the "air" stream increases, the temperature rise found with stoichiometric burning increases, because of the reduced amount of nitrogen participating. At any particular oxygen fraction in the "air", the lower starting temperature gives the greater temperature rise. This is because, in general, specific heats increase with temperature. As the oxidizer approaches standard twenty-one percent oxygen, the three curves also diverge, but below five percent, the temperature rise curves are all closely grouped.

Some of the results from previous sections are portrayed in Figure 17 so as to clarify the trends and values at given operating conditions. It compares the adiabatic flame temperature of stoichiometric methane combustion with the initial temperature. Results are generated for a variety of oxygen percentages in the incoming "air". As expected, the detailed results confirm that the highest flame temperatures occur at the highest oxygen percentages and the highest inlet temperatures.

Finally, Figure 18 vividly illustrates dissociation's dependence on both the composition of the oxidizer and the initial temperature. Graphs of carbon monoxide,

oxygen, and hydrogen are shown. At the lowest initial temperature, dissociation is negligible above the ten percent level of oxygen in the "air". On the other hand, dissociation occurs even at low oxygen percentages when the inlet temperature is at its highest value considered. Near 21% oxygen in the "air", dissociation is significant, for all species and at all inlet temperatures; although the higher initial temperatures generate a proportionally greater increase in dissociated products.

4.4 General Results for CHONS Fuels

To demonstrate the flexibility in AFTC-multifuel, a series of runs were made comparing how the adiabatic flame temperature changes as the fuel's chemical formula changes, for several different equivalence ratios.

4.4.1 Stoichiometric Combustion of CH Fuels over a Variety of Carbon Numbers

Figure 19 illustrates how the flame temperature changes as a function of 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.

4.4.2 Fuel Lean Combustion and Fuel Rich Combustion of CH Fuels

Figures 20 and 21 repeat the section 4.4.1, but for fuel lean and fuel rich equivalence ratios respectively. Following previous results, temperatures are highest for both nondissociated combustion and burning in oxygen.

4.4.3 Stoichiometric Combustion of CHON Fuels

Following the previous two sections, additional results are displayed for more fuels containing oxygen and nitrogen in figure 22. Again, a listing of the fuels used can be found in Appendix E. Once more, the dependency of the flame temperature, and thus dissociation, upon the carbon number is demonstrated. As the carbon number is increased, the flame temperatures approach a single value.

Also, the importance of the LHV arises. For example, the alcohols contain weight adding oxygen. Therefore, it would stand to reason that, for approximately equal LHV's, the alcohols would burn at higher temperatures than standard hydrocarbon, i.e., the paraffins. This does not occur however, because the alcohols have significantly lower LHV's than that of the paraffins. Therefore, even though the extra mass in the molecule would mean a corresponding increase in the heat released during combustion, because the alcohols' heating values are significantly lower than the paraffins', the alcohols follow the same temperature trends as the straight hydrocarbons.

4.5 General Results for Woods and Coals

4.5.1 General Results for Woods

Table 9 and Figure 23 contain similar results for stoichiometric combustion of various woods. These woods contain oxygen. Figure 23 displays curves for hard woods and soft woods. Irrespective of the fuel formula, all the woods burn at approximately the same temperature. Note the woods have a significantly higher adiabatic flame temperature than the other oxygen-bearing fuel, the aliphatic alcohols (section 4.4.3). Both have similar LHV's and carbon to hydrogen ratios. However, the woods all have

double the volume of oxygen in the fuel. Therefore, the woods will have a higher adiabatic flame temperature. Of course, there will be a variety of real world affects that will limit the actual wood flame temperatures, namely necessary phase changes inhibiting the chemical reactions and physical limitations on the fuel and oxidizer mixing.

4.5.1 General Results for Coals

Figure 24 contains similar results for coal combustion, the chemical formulas of which can be found in Appendix E. These are also tabulated in Table 9. Although coal has a higher energy density than wood, it does not burn as hot, adiabatically, because it does not contain nearly as much oxygen. Furthermore, small amounts of nitrogen and even sulfur are present in the coal. As has been shown previously, this will further depress the flame temperatures.

4.6 Comparison with Other Methods

An alternative method for solving the flame temperature and product composition is to use a Newton-Raphson Iteration of the unknown variables from section 3.1. This is the method used in both the well known programs by Turns (2001) and Gordon-McBride. It is also implemented in Ferguson and Kirkpatrick (2001). This method may offer a more direct solution to the equations, but at the cost of guaranteed convergence, Campbell (1979). In addition to the dissociated species accounted for in AFTC, these programs also account for H, NO, O, OH, and N.

A tabulated comparison of these programs with AFTC is given in Table 10. For completeness, Goodger's (1977) temperature predictions are included as well. 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 11 then recalculates the results of Table 10 to give each program's percent difference in temperature, relative to AFTC.

Both Tables 10 and 11 provide results for a sampling of different fuel types. 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. With the sole exception of Gordon and McBride's result for methane, 1.68%, AFTC showed very good agreement with all the programs for the standard hydrocarbons of less than one percent. 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 several possible explanations for the differing adiabatic flame temperatures predicted by each program. Primarily, one must consider the number of significant digits used in the calculation. For example, for standard air consisting of 21% oxygen, there are 3.762 moles of nitrogen for every mole of oxygen in the air. However, this value is often shortened to 3.76 moles. This seemingly negligible difference can result in a 10K difference in the final temperature. Additionally, depending on the table

used, different programs may use slightly different physical quantities. And of course,

each program may define convergence of its numerical iterations differently.

CHAPTER FIVE

CONCLUSIONS

The mathematical background and algorithms of the AFTC computer code that enable the adiabatic flame temperature and product composition to be calculated have been described. Complexities included: type of fuel, amount of oxidant, type of oxidant (air or oxygen), amount of oxygen in the "air", inlet temperatures of the fuel and oxidant streams, and inclusion or not of dissociation effects. The most complicated case required nested half-interval searches for temperature and species. Although any fuel can be investigated with the methodology and computer code simulation described herein, the emphasis has been on the fuel methane, burning under stoichiometric conditions.

Additionally, flame temperature and product species composition computations have been made of fuel combustion with oxygen-deficient air, with both fuel and "air" entering at elevated temperatures, and at different equivalence ratios and pressures. These concepts of high inlet temperature (up to 1500K) air with reduced oxygen concentrations (down to 2.5% by volume) are paramount in the new technology of "High Temperature Air Combustion" for efficient low pollution furnace operation. Therefore, some combustion trends related to this were discussed.

Finally, a comparison with other methods and programs was given. Despite the differences in dissociation complexity, there was little variation of the adiabatic flame temperature from different methods. As one would expect, Goodger's (1977) results were very similar to AFTC's results. Furthermore, AFTC showed close agreement with

the common programs Turns (2001) and Gordon and McBride (Glassman, 1987). Throughout, results showing the accuracy, robustness and versatility of the code have been given, and the associated combustion trends were discussed.

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Appendix A

Tables

Table 1. Temperature and Molar (volume) fractions of product species
for stoichiometric oxygen-fuel flames
[ND = no dissociation, WD = with dissociation]

Fuel		Temperature	Molar Fraction of					
		Degrees K	CO	CO_2	H_2O	N_2	O_2	H_2
Methane	ND	5264		0.333	0.667			
CH_4	WD	3378	0.202	0.073	0.406		0.174	0.145
Propane	ND	5595		0.429	0.571			
C_3H_8	WD	3441	0.261	0.084	0.329		0.196	0.130
Butane	ND	5637		0.444	0.556			
C_4H_{10}	WD	3447	0.270	0.086	0.318		0.198	0.127
Decane	ND	5722		0.476	0.524			
$C_{10}H_{22}$	WD	3459	0.288	0.091	0.296		0.204	0.120

Table 2. Temperature and Molar (volume) fractions of product species
for stoichiometric air-fuel flames
[ND = no dissociation, WD = with dissociation]

Fuel		Temperature	Molar Fraction of					
		Degrees K	CO	CO_2	H_2O	N_2	O_2	H_2
Methane	ND	2326		0.095	0.190	0.715		
CH_4	WD	2244	0.009	0.085	0.185	0.710	0.006	0.004
Propane	ND	2393		0.116	0.155	0.729		
C_3H_8	WD	2288	0.013	0.103	0.150	0.723	0.008	0.003
Butane	ND	2399		0.120	0.149	0.731		
C_4H_{10}	WD	2291	0.013	0.105	0.145	0.725	0.008	0.003
Decane	ND	2410		0.126	0.139	0.735		
$C_{10}H_{22}$	WD	2298	0.014	0.111	0.134	0.729	0.009	0.003

Table 3. Temperature and Molar (volume) fractions of product species
for stoichiometric methane flames in oxygen-enriched and oxygen-deficient "air" at 298K inlet conditions
[ND = no dissociation, WD = with dissociation]

Oxygen Volume Percent		Temperature	Molar Fraction of					
		Degrees K	CO	CO_2	H_2O	N_2	O_2	H_2
10%	ND	1437		0.048	0.095	0.857		
	WD	1437	0.000	0.048	0.095	0.857	0.000	0.000
15%	ND	1873		0.070	0.140	0.791		
	WD	1863	0.001	0.069	0.139	0.790	0.001	0.000
21%	ND	2326		0.095	0.190	0.715		
	WD	2244	0.009	0.085	0.185	0.710	0.006	0.004
25%	ND	2594		0.111	0.222	0.667		
	WD	2423	0.019	0.090	0.212	0.658	0.013	0.008
30%	ND	2898		0.130	0.261	0.609		
	WD	2591	0.035	0.092	0.240	0.594	0.025	0.014

Table 4. Temperature and Molar (volume) fractions of product species
for stoichiometric methane flames in oxygen-enriched and oxygen-deficient "air" at 1000K inlet conditions
[ND = no dissociation, WD = with dissociation]

Oxygen Volume Percent		Temperature	Molar Fraction of					
		Degrees K	CO	CO_2	H_2O	N_2	O_2	H_2
10%	ND	1992		0.048	0.095	0.857		
	WD	1976	0.002	0.046	0.094	0.856	0.001	0.001
15%	ND	2399		0.070	0.140	0.791		
	WD	2311	0.009	0.060	0.135	0.785	0.007	0.004
21%	ND	2827		0.095	0.190	0.715		
	WD	2579	0.027	0.066	0.175	0.701	0.019	0.011
25%	ND	3081		0.111	0.222	0.667		
	WD	2708	0.041	0.067	0.198	0.647	0.029	0.018
30%	ND	3370		0.130	0.261	0.609		
	WD	2836	0.058	0.067	0.222	0.582	0.043	0.028

Table 5. Temperature and Molar (volume) fractions of product species
for stoichiometric methane flames in oxygen-deficient "air" for 298K inlet conditions
[ND = no dissociation, WD = with dissociation]

Oxygen Volume Percent		Temperature	Molar Fraction of					
		Degrees K	CO	CO_2	H_2O	N_2	O_2	H_2
2.5%	ND	618		0.012	0.025	0.963		
	WD	618	0.000	0.012	0.025	0.963	0.000	0.000
5.0%	ND	925		0.024	0.049	0.927		
	WD	925	0.000	0.024	0.049	0.927	0.000	0.000
7.5%	ND	1193		0.036	0.072	0.892		
	WD	1193	0.000	0.036	0.072	0.892	0.000	0.000
10.0%	ND	1437		0.048	0.095	0.857		
	WD	1437	0.000	0.048	0.095	0.857	0.000	0.000
12.5%	ND	1663		0.059	0.118	0.824		
	WD	1661	0.000	0.059	0.118	0.823	0.000	0.000
15.0%	ND	1873		0.070	0.140	0.791		
	WD	1863	0.001	0.069	0.139	0.790	0.001	0.000
21.0%	ND	2326		0.095	0.190	0.715		
	WD	2244	0.009	0.085	0.185	0.710	0.006	0.004

Table 6. Temperature and Molar (volume) fractions of product species
for stoichiometric methane flames in oxygen-deficient "air" for 1000K inlet conditions
[ND = no dissociation, WD = with dissociation]

Oxygen Volume Percent		Temperature Degrees K	Molar Fraction of CO	CO_2	H_2O	N_2	O_2	H_2
2.5%	ND	1264		0.012	0.025	0.963		
	WD	1264	0.000	0.012	0.025	0.963	0.000	0.000
5.0%	ND	1525		0.024	0.049	0.927		
	WD	1525	0.000	0.024	0.049	0.927	0.000	0.000
7.5%	ND	1767		0.036	0.072	0.892		
	WD	1764	0.000	0.036	0.072	0.891	0.000	0.000
10.0%	ND	1992		0.048	0.095	0.857		
	WD	1976	0.002	0.046	0.094	0.856	0.001	0.001
12.5%	ND	2202		0.059	0.118	0.824		
	WD	2159	0.004	0.054	0.115	0.821	0.003	0.002
15.0%	ND	2399		0.070	0.140	0.791		
	WD	2311	0.009	0.060	0.135	0.785	0.007	0.004
21.0%	ND	2827		0.095	0.190	0.715		
	WD	2579	0.027	0.066	0.175	0.701	0.019	0.011

Table 7. Temperature and Molar (volume) fractions of product species
for stoichiometric methane flames in oxygen-deficient "air" for 1250K inlet conditions
[ND = no dissociation, WD = with dissociation]

Oxygen Volume Percent		Temperature Degrees K	Molar Fraction of CO	CO_2	H_2O	N_2	O_2	H_2
2.5%	ND	1476		0.012	0.025	0.963		
	WD	1476	0.000	0.012	0.025	0.963	0.000	0.000
5.0%	ND	1730		0.024	0.049	0.927		
	WD	1727	0.000	0.024	0.049	0.927	0.000	0.000
7.5%	ND	1965		0.036	0.072	0.892		
	WD	1953	0.001	0.035	0.072	0.891	0.001	0.001
10.0%	ND	2185		0.048	0.095	0.857		
	WD	2148	0.004	0.044	0.093	0.855	0.003	0.002
12.5%	ND	2391		0.059	0.118	0.824		
	WD	2311	0.008	0.050	0.114	0.819	0.006	0.003
15.0%	ND	2584		0.070	0.140	0.791		
	WD	2444	0.015	0.054	0.132	0.782	0.010	0.006
21.0%	ND	3003		0.095	0.190	0.715		
	WD	2683	0.034	0.058	0.170	0.697	0.025	0.015

Table 8. Temperature and Molar (volume) fractions of product species
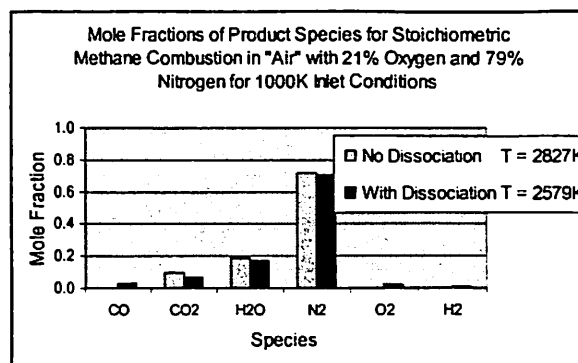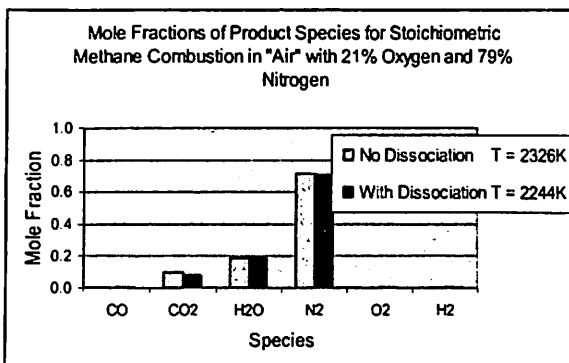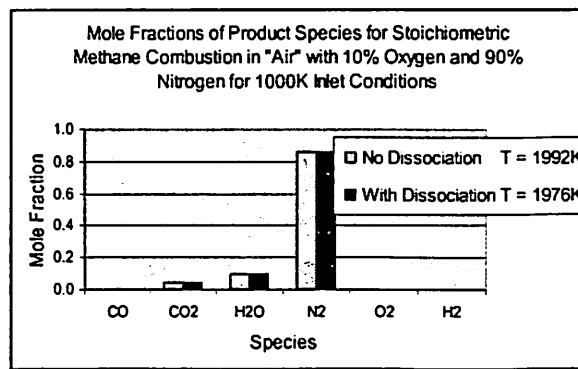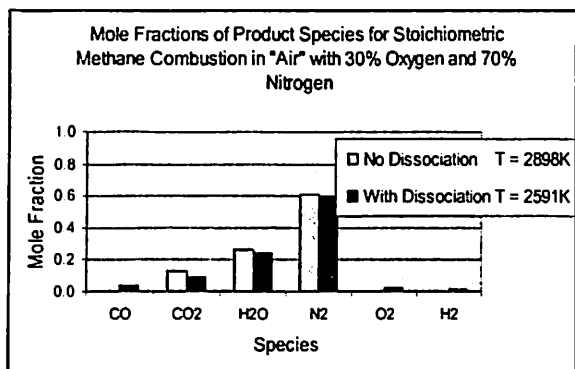for stoichiometric methane flames in oxygen-deficient "air" for 1500K inlet conditions
[ND = no dissociation, WD = with dissociation]

Oxygen Volume Percent		Temperature		Molar Fraction of					
		Degrees K	CO	CO_2	H_2O	N_2	O_2	H_2
2.5%	ND	1684		0.012	0.025	0.963		
	WD	1683	0.000	0.012	0.025	0.963	0.000	0.000
5.0%	ND	1931		0.024	0.049	0.927		
	WD	1923	0.001	0.024	0.048	0.926	0.001	0.000
7.5%	ND	2161		0.036	0.072	0.892		
	WD	2132	0.003	0.033	0.071	0.890	0.002	0.001
10.0%	ND	2376		0.048	0.095	0.857		
	WD	2307	0.007	0.040	0.092	0.853	0.005	0.003
12.5%	ND	2578		0.059	0.118	0.824		
	WD	2450	0.013	0.045	0.111	0.816	0.009	0.005
15.0%	ND	2767		0.070	0.140	0.791		
	WD	2568	0.021	0.048	0.129	0.779	0.015	0.009
21.0%	ND	3179		0.095	0.190	0.715		
	WD	2782	0.042	0.051	0.164	0.693	0.031	0.020

Table 9. Adiabatic flame temperature(K) vs. fuel carbon number of stoichiometric flames
in dry standard air and oxygen
[ND = no dissociation, WD = with dissociation]

Fuel Category	Fuel Name	Carbon Number	ND Air	WD Air	ND O_2	WD O_2
SOFTWOODS	white cedar	0.18	2745	2497	5036	3272
	douglas fir	0.20	2697	2470	5142	3296
	pitch pine	0.21	2644	2445	5374	3376
	white pine	0.20	2744	2496	5199	3312
	yellow pine	0.19	2683	2466	5141	3310
HARDWOODS	white ash	0.18	2692	2470	5018	3274
	white birch	0.19	2729	2489	5062	3280
	Maple	0.20	2702	2471	5083	3273
	black oak	0.19	2773	2511	5055	3273
	red oak	0.18	2732	2492	5055	3282
	white oak	0.19	2710	2479	5062	3281
COALS	meta-anthracite	0.90	2468	2316	6610	3517
	Anthracite	0.72	2491	2335	6509	3545
	Semianthracite	0.64	2478	2329	6400	3540
	low-volatile bituminous	0.61	2476	2329	6341	3526
	medium-volatile bituminous	0.57	2447	2311	6207	3492
	high-volatile A bituminous	0.53	2417	2316	6132	3480
	high-volatile B bituminous	0.52	2389	2291	6000	3444
	high-volatile C bituminous	0.51	2446	2273	5906	3419
	subbituminous A	0.50	2447	2309	5964	3423
	subbituminous B	0.46	2425	2296	5803	3387
	subbituminous C	0.50	2426	2295	5850	3382
	lignite	0.48	2436	2301	5819	3376

Table 10. 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&G	G&M
Methane	CH4	2248	2247	2226	2227	2210
Propane	C3H8	2274	2289	2267	2268	-
Heptane	C7H16	2281	2298	2274	-	2290
Acetylene	C2H2	2558	2583	2539	2540	-
Methanol	CH3OH	2229	2243	2221	-	-
Hydrogen	H2	2419	2444	2382	2383	2400
Carbon Monoxide	CO	2364	2399	2383	-	2400
Cyanogen	C2N2	2588	-	2594	2596	-

Table 11. 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&G	G&M
Methane	CH4	0	-0.03	-0.97	-0.92	-1.68
Propane	C3H8	0	0.67	-0.30	-0.26	-
Heptane	C7H16	0	0.76	-0.30	-	0.40
Acetylene	C2H2	0	0.99	-0.73	-0.69	-
Methanol	CH3OH	0	0.63	-0.35	-	-
Hydrogen	H2	0	1.05	-1.52	-1.47	-0.77
Carbon Monoxide	CO	0	1.46	0.78	-	1.50
Cyanogen	C2N2	0	-	0.21	0.29	-

Appendix B

Figures
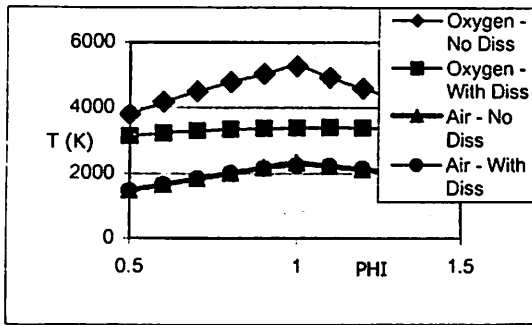
Figure 1. Adiabatic flame temperature for methane
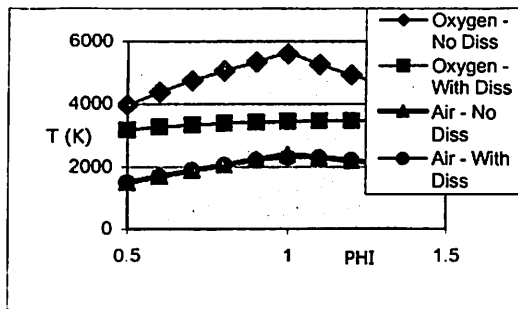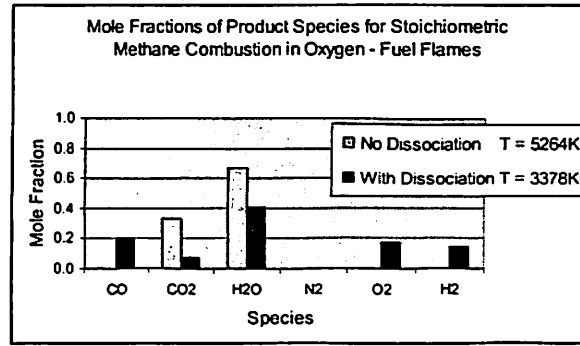
Figure 2. Adiabatic flame temperature for propane
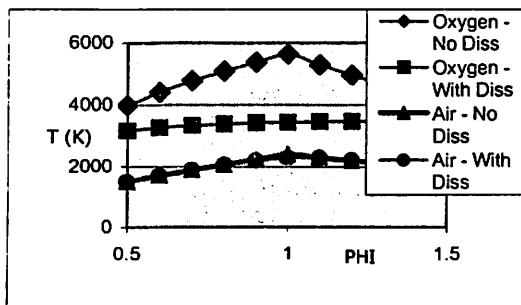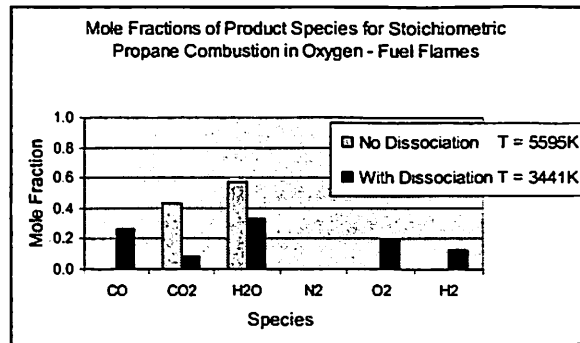
Figure 3. Adiabatic flame temperature for butane
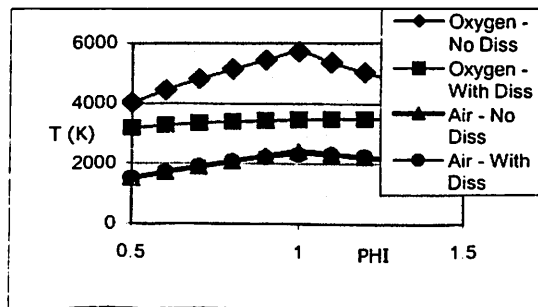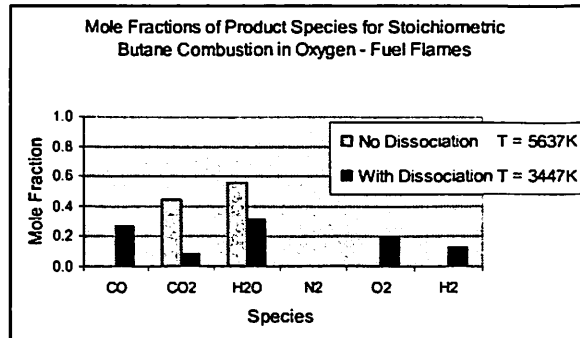
Figure 4. Adiabatic flame temperature for decane
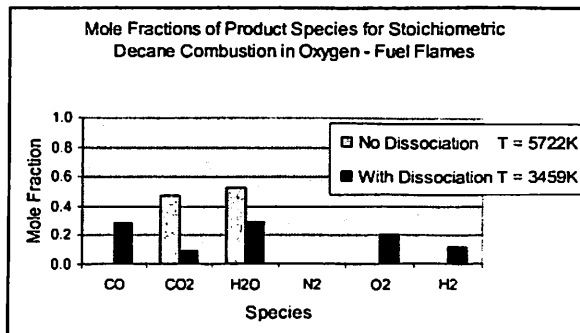
Figure 5.   Temperature and Molar (volume) fractions of product species; for stoichiometric oxygen-fuel flames for methane, propane, butane, and decane

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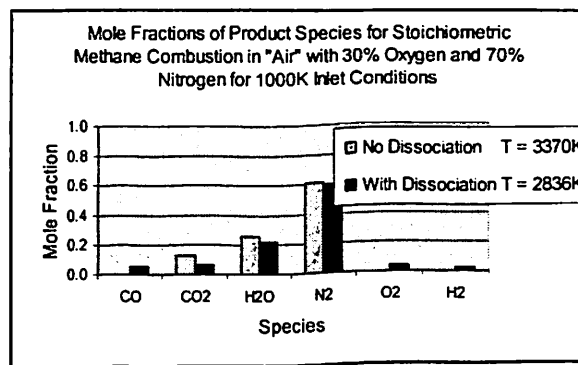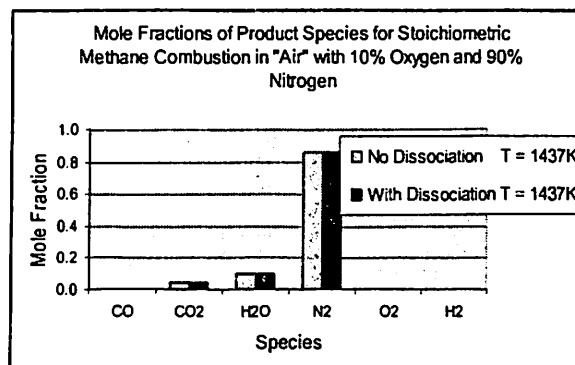
Figure 6. Temperature and Molar (volume) fractions of product species for stoichiometric methane flames in oxygen-enriched and oxygen-deficient "air"; for 10%, 21%, and 30% oxygen in the "air"; with nitrogen comprising the other components, for fuel and oxidizer inlet conditions of 298K

Figure 7. Temperature and Molar (volume) fractions of product species for stoichiometric methane flames in oxygen-enriched and oxygen-deficient "air"; for 10%, 21%, and 30% oxygen in the "air"; with nitrogen comprising the other components; for fuel and oxidizer inlet conditions of 1000K
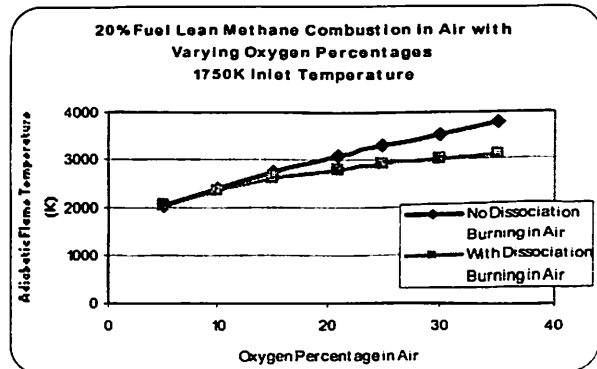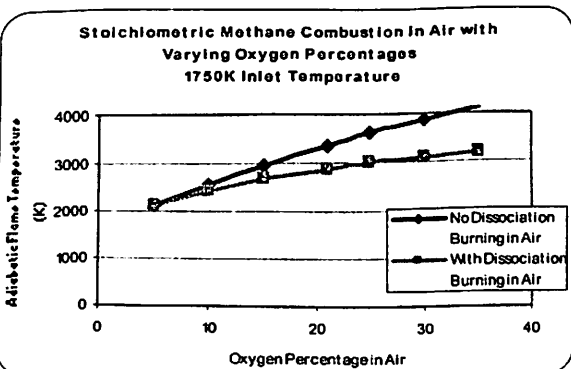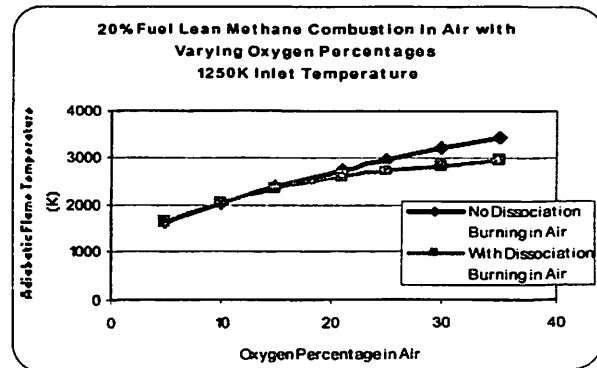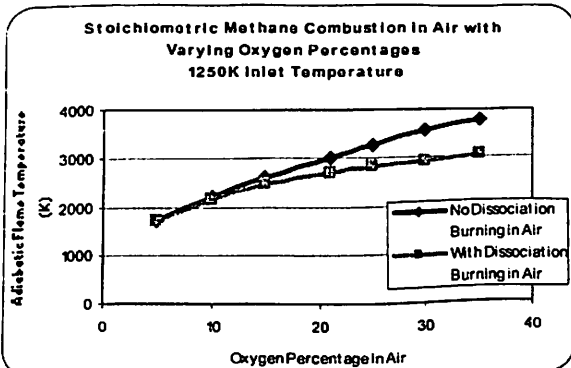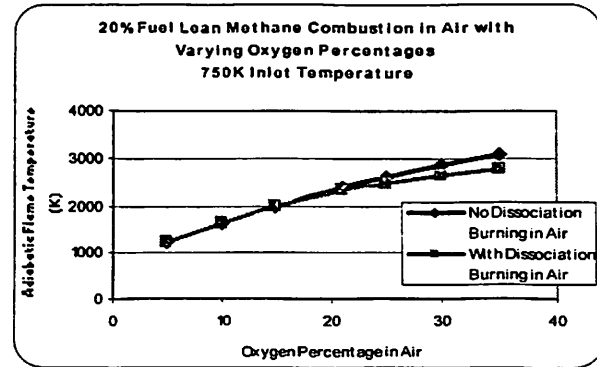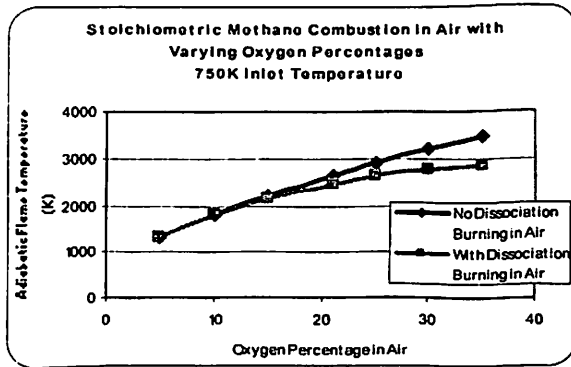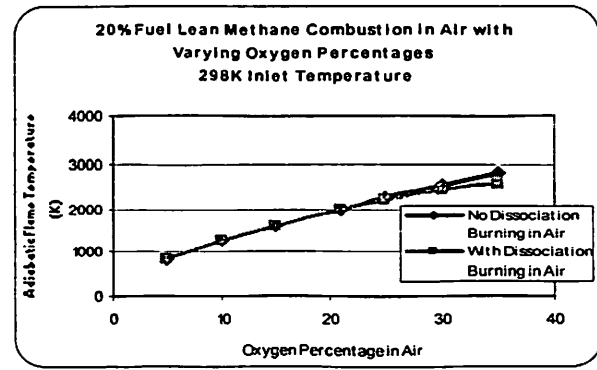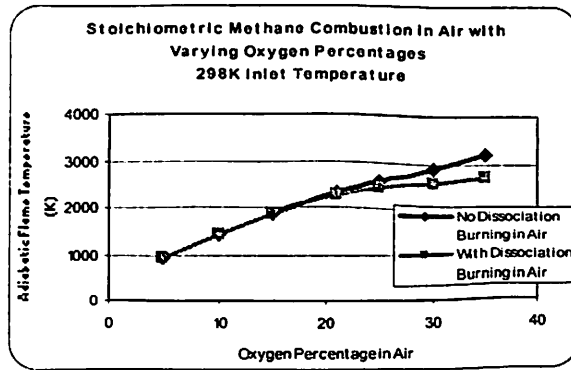
Figure 8. Flame Temperature for Methane Burning in Stoichiometric "Air", for Elevated Fuel and Oxidizer Inlet Temperatures

Figure 9. Flame Temperature for Methane Burning in 20% Fuel Lean "Air", for Elevated Fuel and Oxidizer Inlet Temperatures
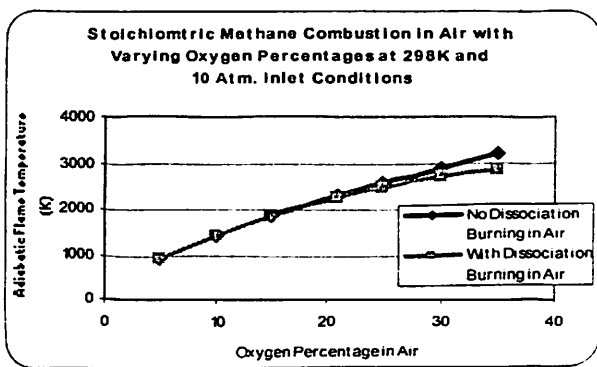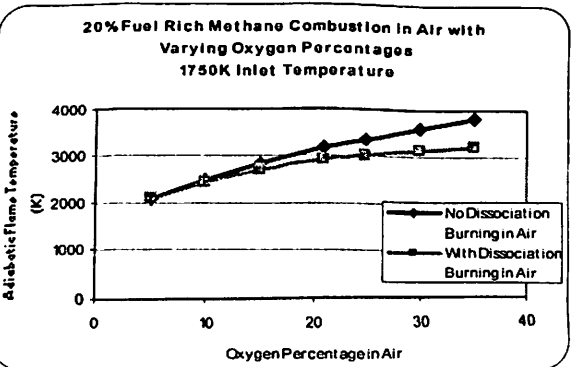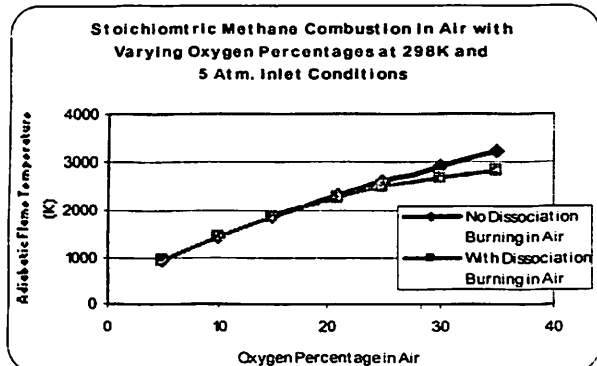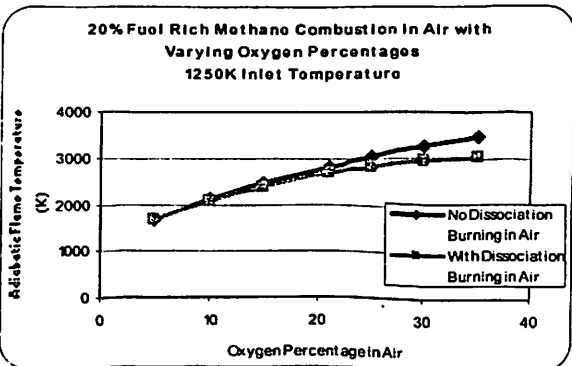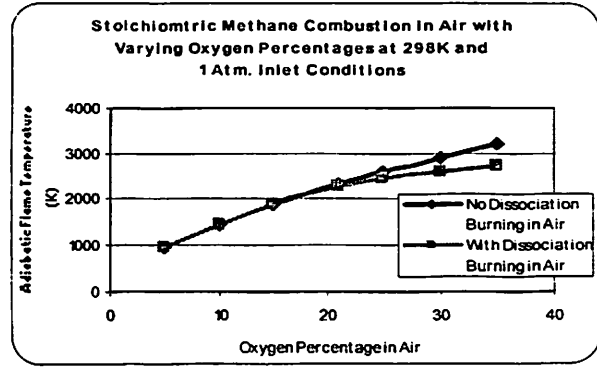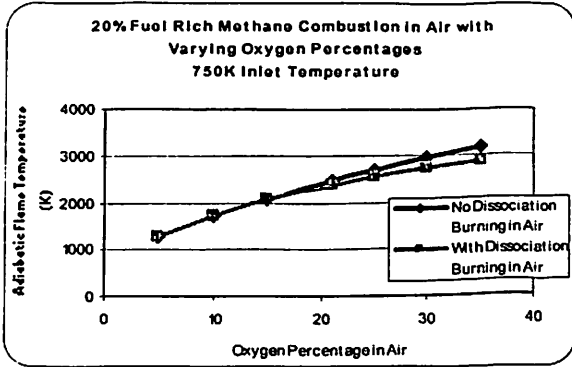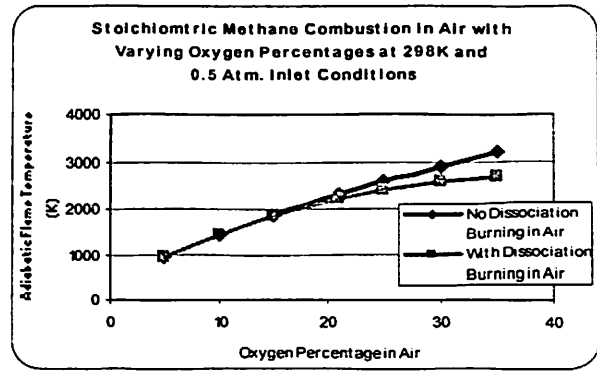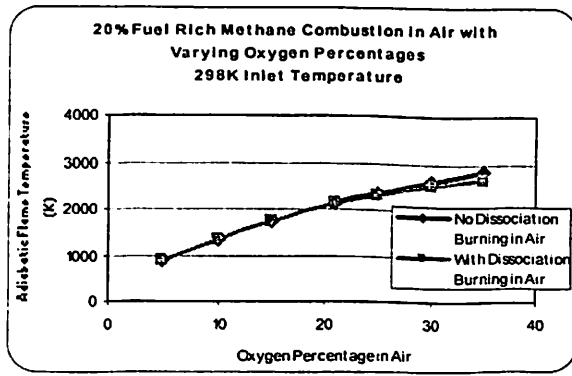
Figure 10. Flame Temperature for Methane Burning in 20% Fuel Rich "Air", for Elevated Fuel and Oxidizer Inlet Temperatures

Figure 11. Flame Temperature for Methane Burning in Stoichiometric "Air", for Varying Combustion Pressures
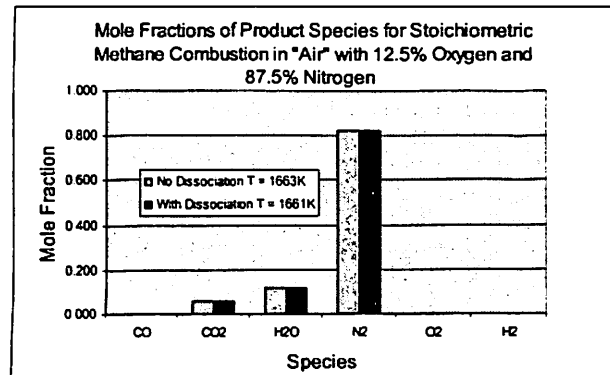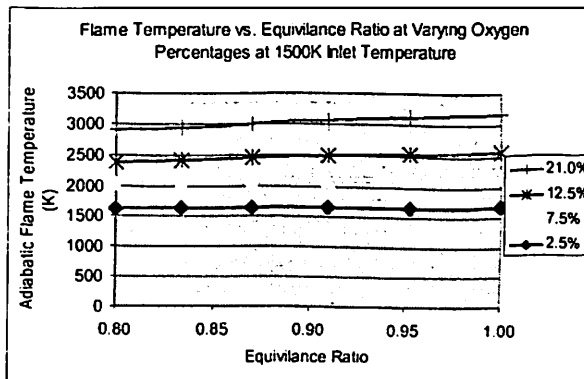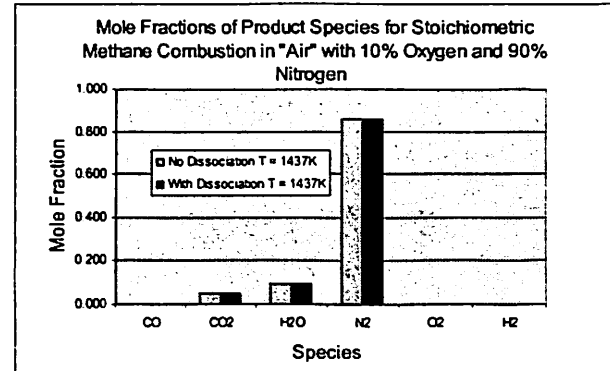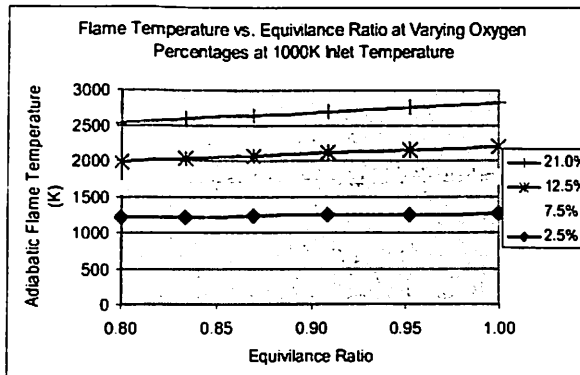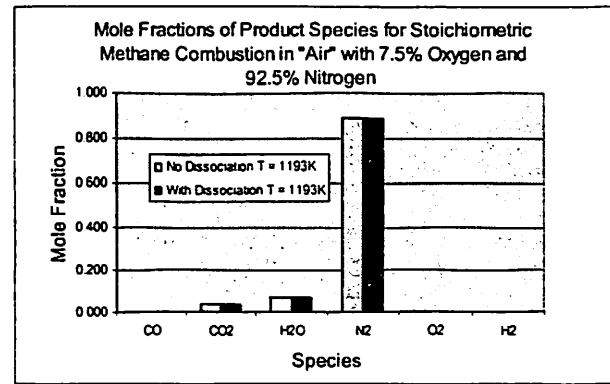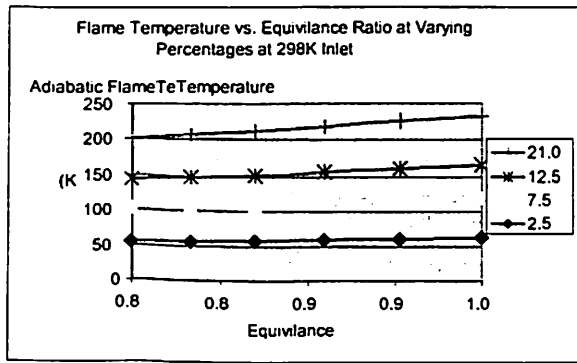
Figure 12. Flame Temperature at Different Fuel Lean Ratios for a Variety of Oxygen-Deficient "Air" Conditions, for Different Inlet Temperatures
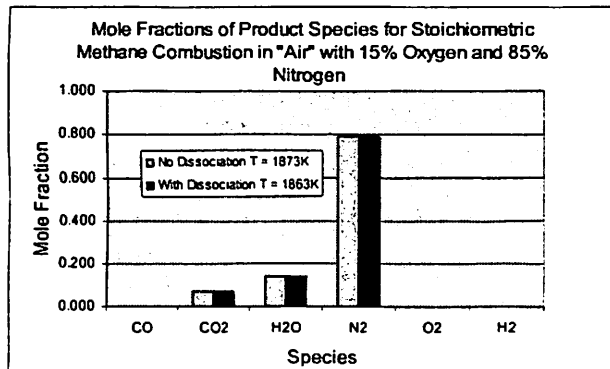
Figure 13. Flame Temperature and Product Species for Methane Burning in Oxygen-Deficient "Air", for Fuel and Oxidizer Inlet Conditions of 298K
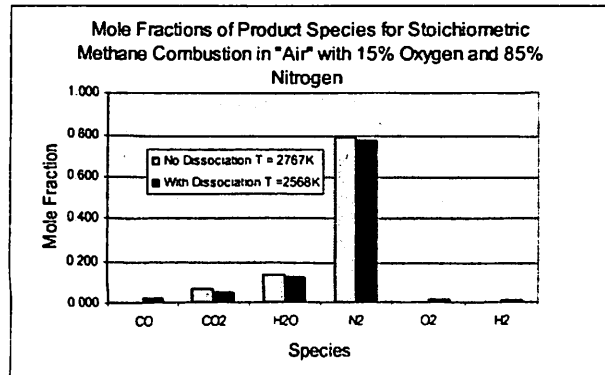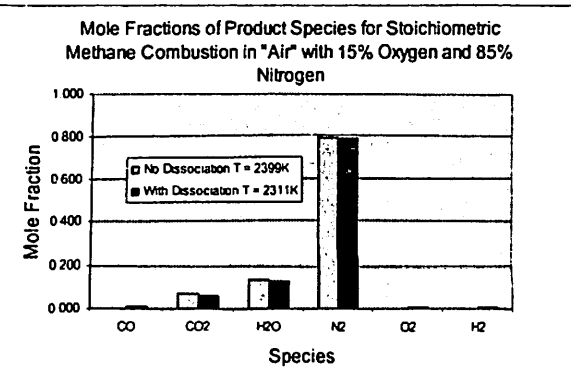
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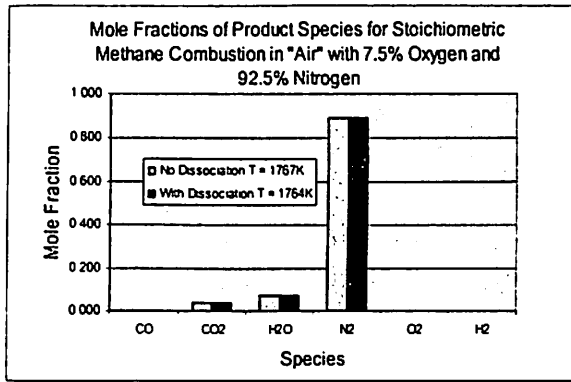
Figure 14. Flame Temperature and Product Species for Methane Burning in Oxygen-Deficient "Air", for Fuel and Oxidizer Inlet Conditions of 1000K

Figure 15. Flame Temperature and Product Species for Methane Burning in Oxygen-Deficient "Air", for Fuel and Oxidizer Inlet Conditions of 1500K
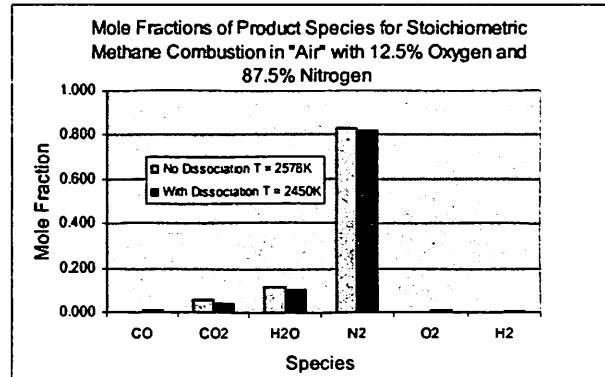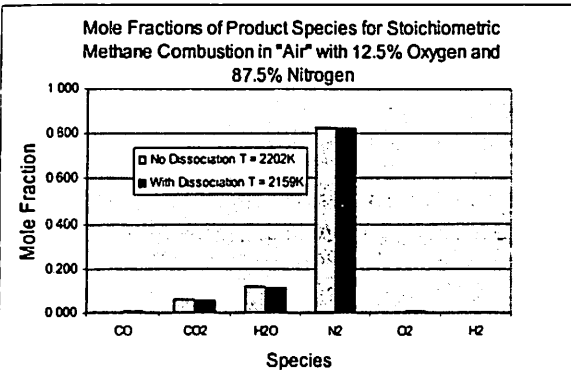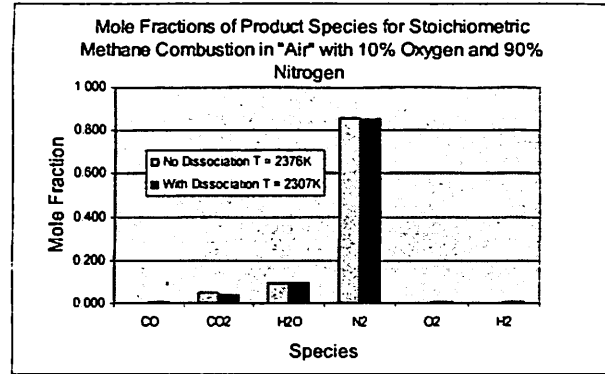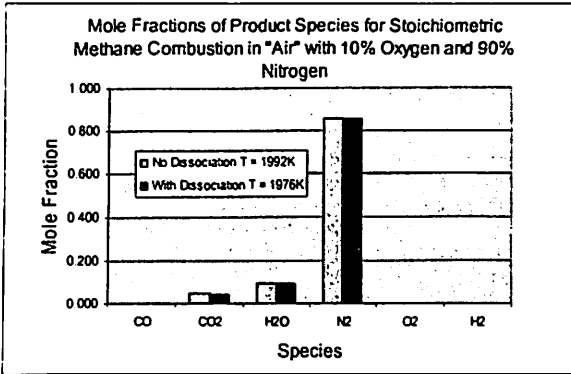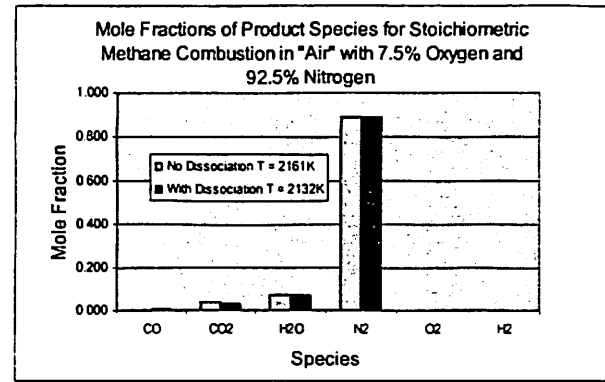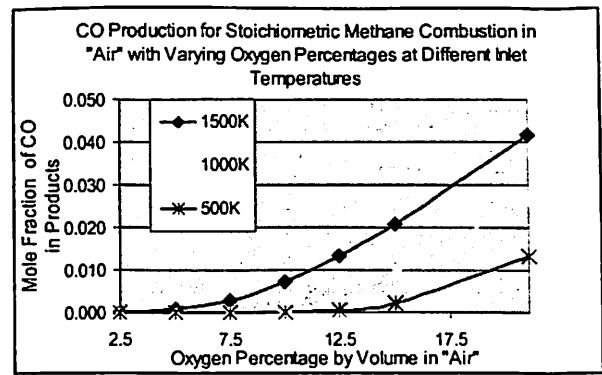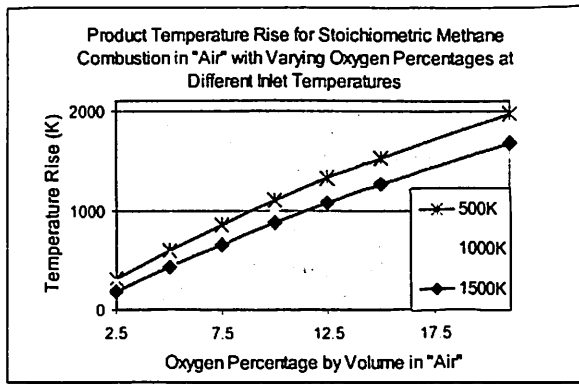
Figure 16. Flame Temperature Rise Across Varying Oxygen Percentages For Different Fuel and Oxidizer Inlet Conditions
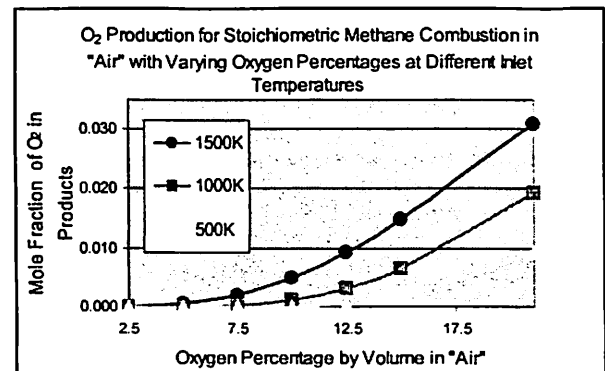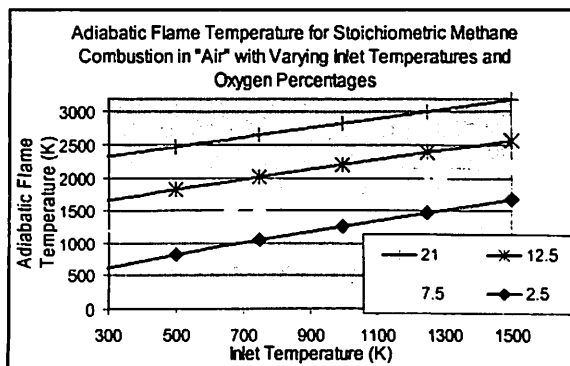
Figure 17. Adiabatic Flame Temperature Across Varying Inlet Temperatures For Different Oxygen Percentages of "Air"
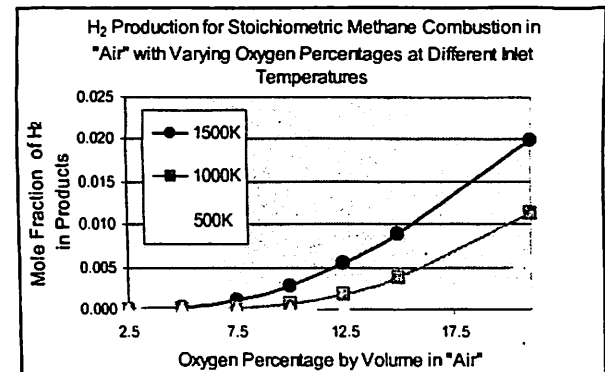
Figure 18. Mole Fraction in Product Stream for Different Oxygen Percentages of "Air" at Different Inlet Temperatures, for Carbon Monoxide, Oxygen, and Hydrogen
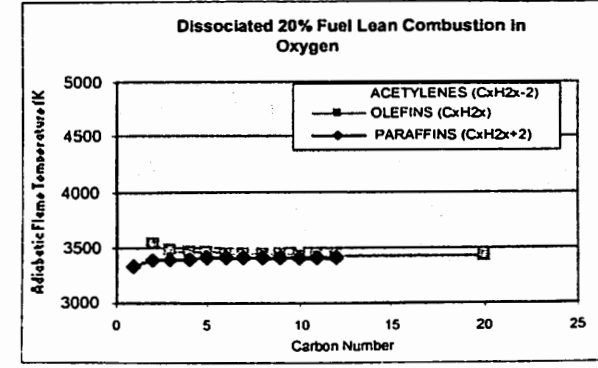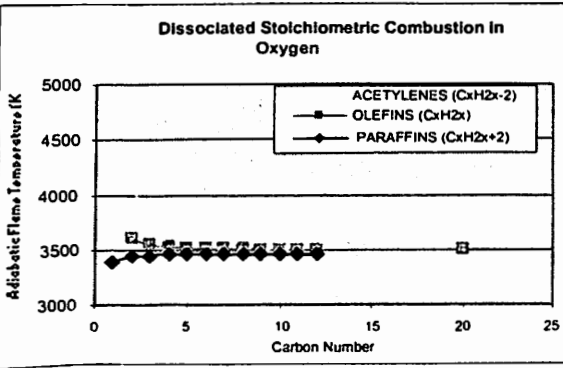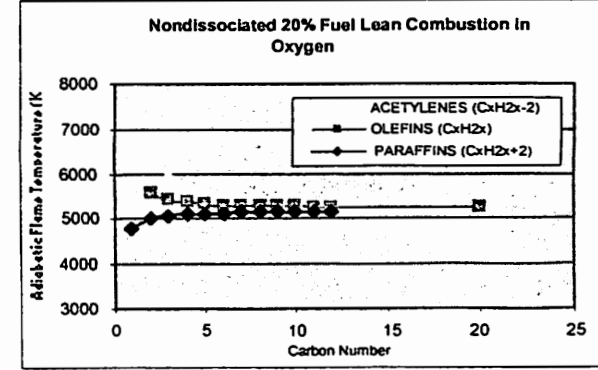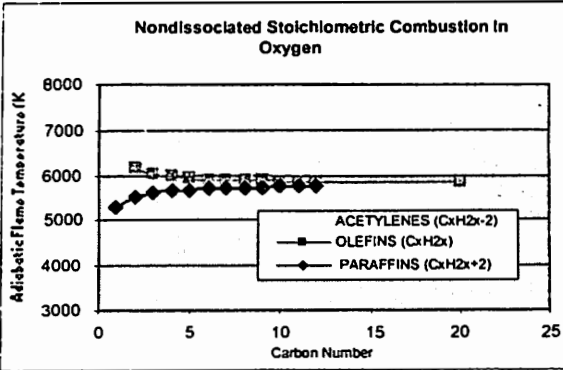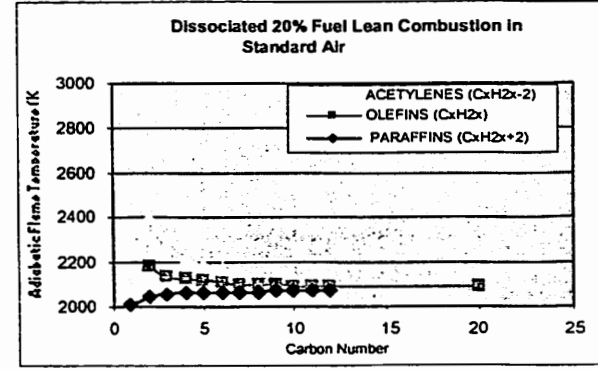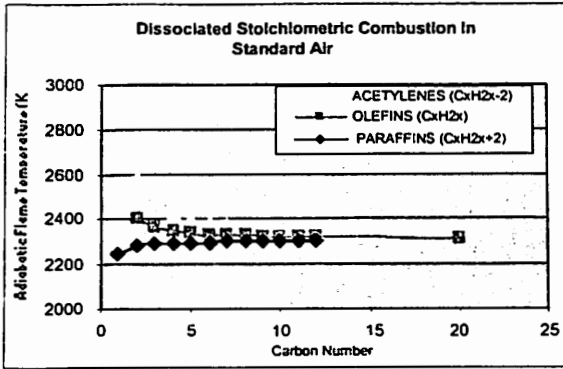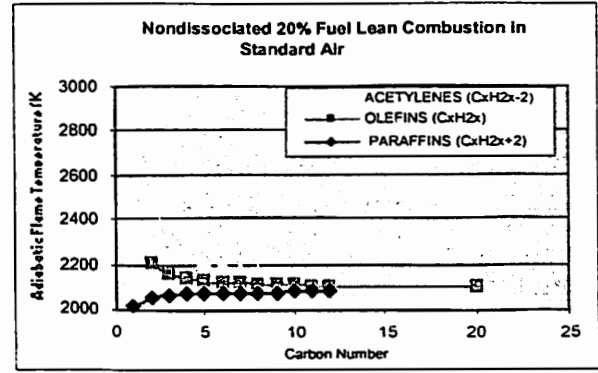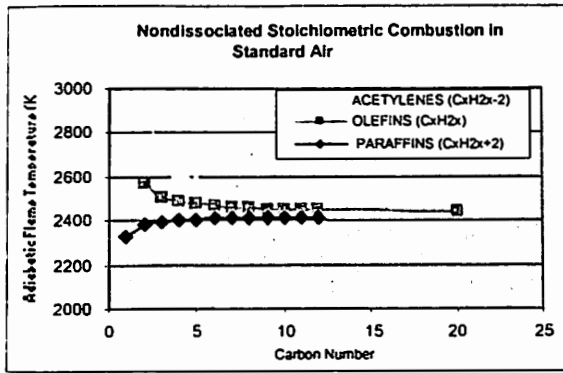
Figure 19. Stoichiometric Adiabatic Flame Temperature as a Function of the Fuel Carbon Number

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

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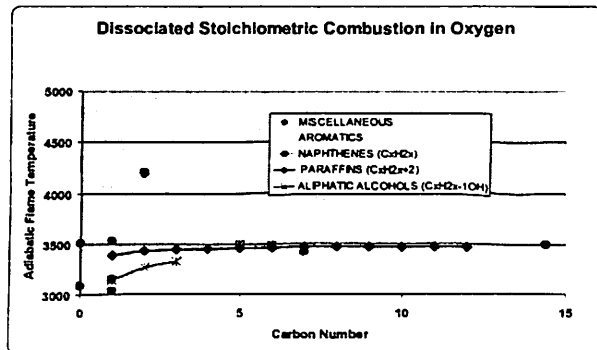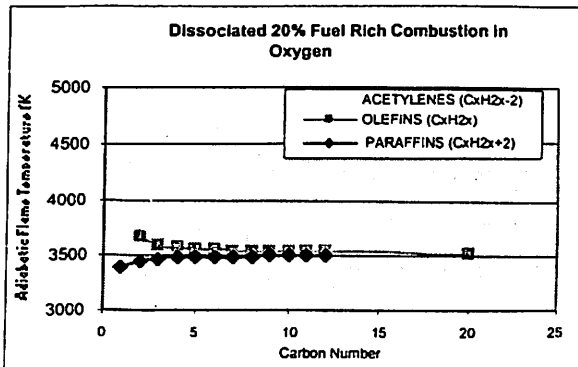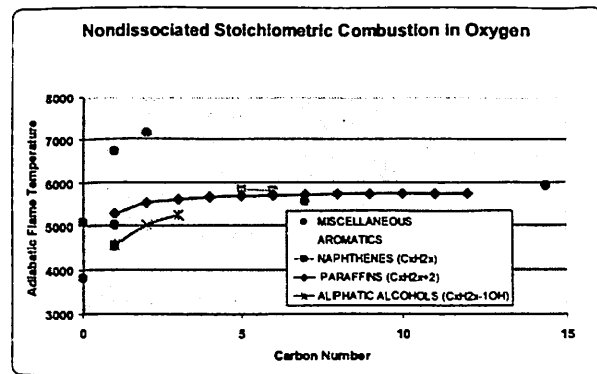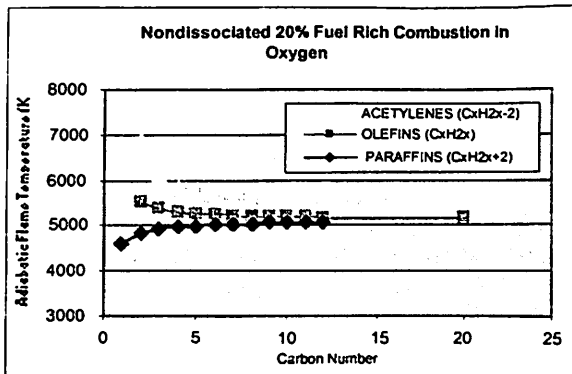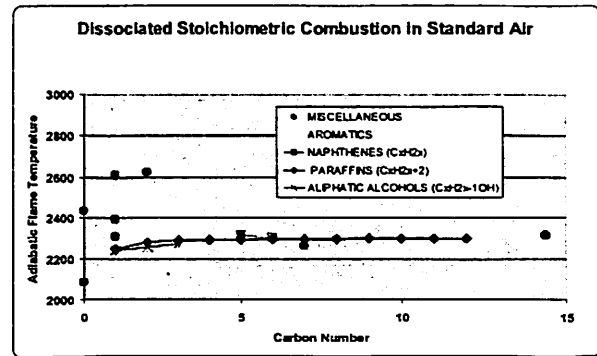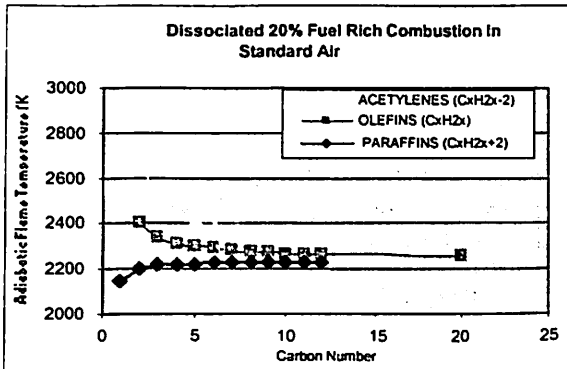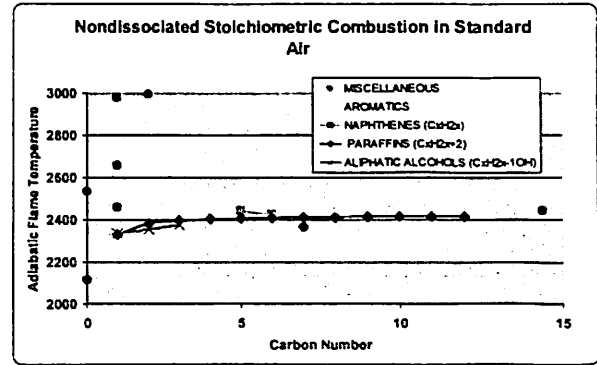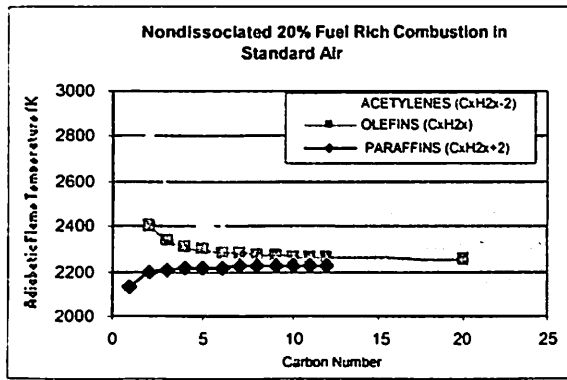
Figure 21. 20% Fuel Rich Adiabatic Flame Temperature as a Function of the Fuel Carbon Number

Figure 22. Stoichiometric Adiabatic Flame Temperature as a Function of the Fuel Carbon Number

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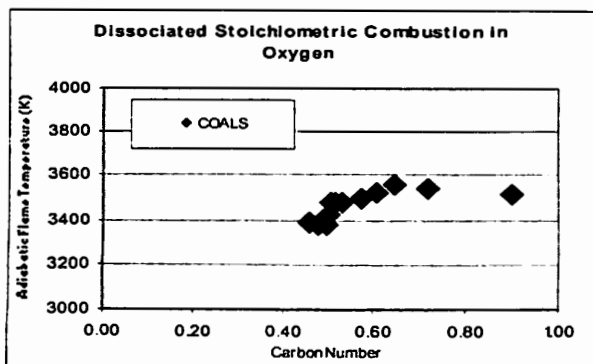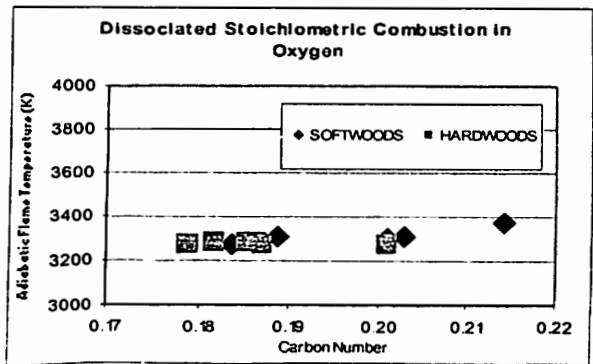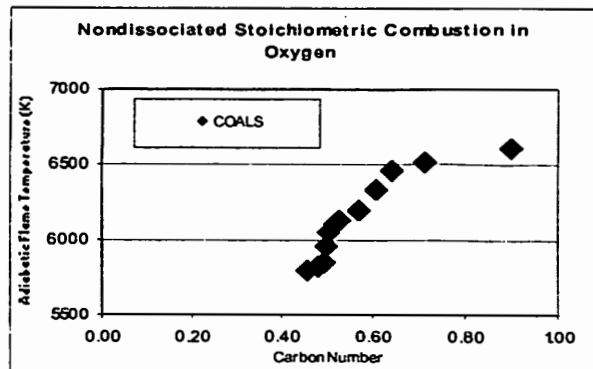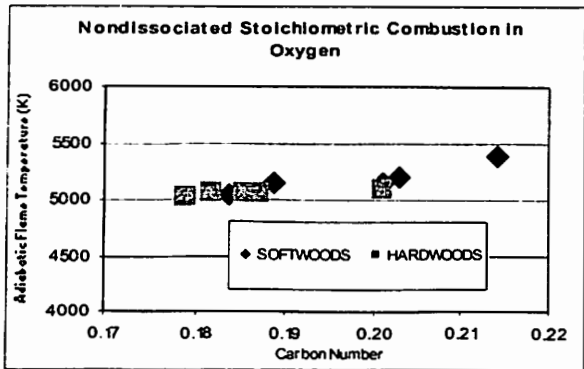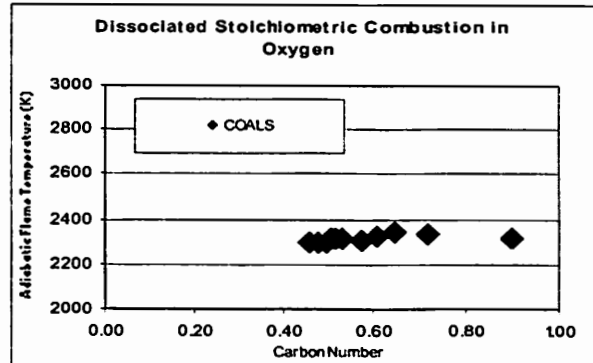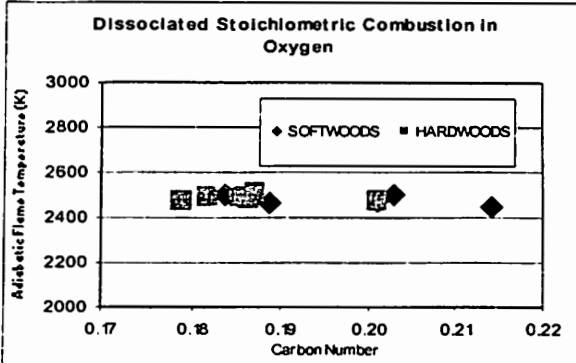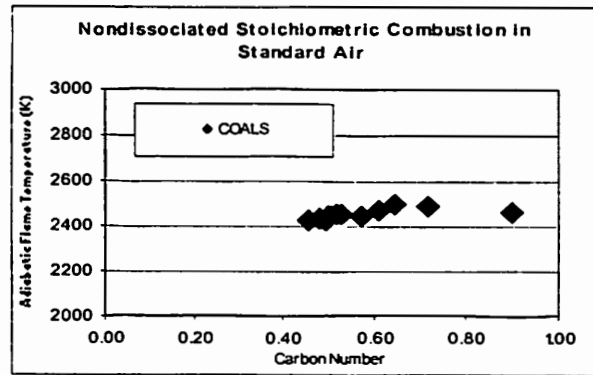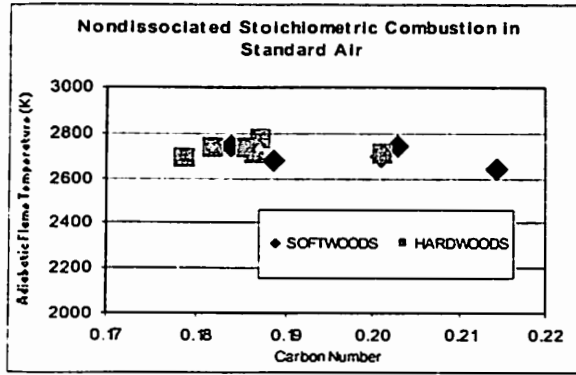
Figure 23. Stoichiometric Adiabatic Flame Temperature For Soft and Hard Woods

Figure 24. Stoichiometric Adiabatic Flame Temperature For Selected Coals

Appendix C

Curve Fit Calculations

In using the JANAF Thermochemical Tables, JANAF (1986), to calculate curve fits for sulfur dioxide, special care had to be taken. The values listed in JANAF required a unit conversion and their reference had to be shifted from 298.15K to 0K. This leads to a reference enthalpy of 10552 kJ/kmol at 298.15K. At the following temperatures, the following enthalpies were adjusted by the reference enthalpy and were then used to calculate the curve fit constants through a simple matrix inversion.

Temp. (K)	Enthalpy (kJ/kg-mol)
500	8758
1100	39914
1600	68123
2500	120559
4000	210145
5500	301534

$$
\begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 1 & T_1 & \ln(T_1) \\ 1 & T_2 & \ln(T_2) \\ 1 & T_3 & \ln(T_3) \end{pmatrix}^{-1} \cdot \begin{pmatrix} h_1 + \text{ref} \\ h_2 + \text{ref} \\ h_3 + \text{ref} \end{pmatrix}
$$

So, for low and high temperature ranges, the values of A, B, and C for sulfur dioxide are:

Species	A	B	C
SO_2 (400K-1600K)	37548	62.38	-7953.4
SO_2 (1600K-6000K)	65565	63.45	-11897

Where again, the enthalpy equation is $h = A + BT + C\ln(T)$.

This curve is plotted in the graph below, along with data points from the JANAF tables. As one can see, the curve fit shows good agreement with the source data.

Comparison of the AFTC Sulfur Dioxide Enthalpy Curve Fit with JANAF Data
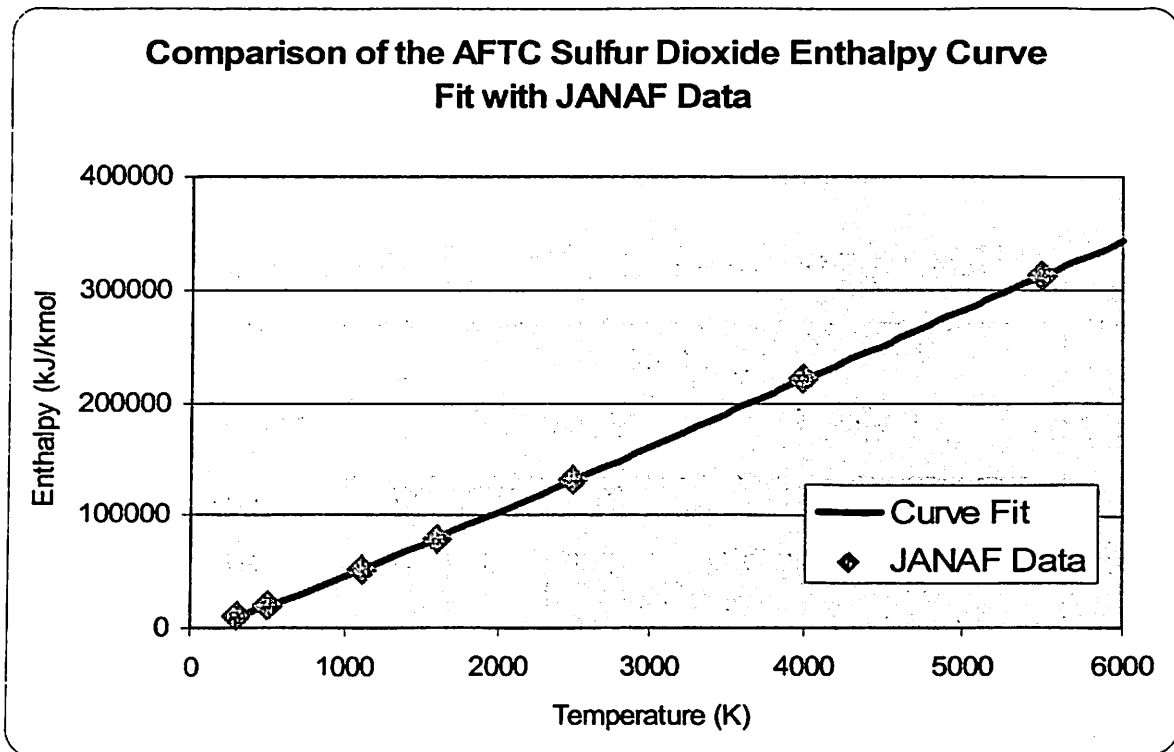
Similarly, the curve fits for the other species were also plotted. The solid symbols are the curve fit points. The empty symbols are adjusted JANAF data.

Comparison of the AFTC Enthalpy Curve Fits with JANAF Data
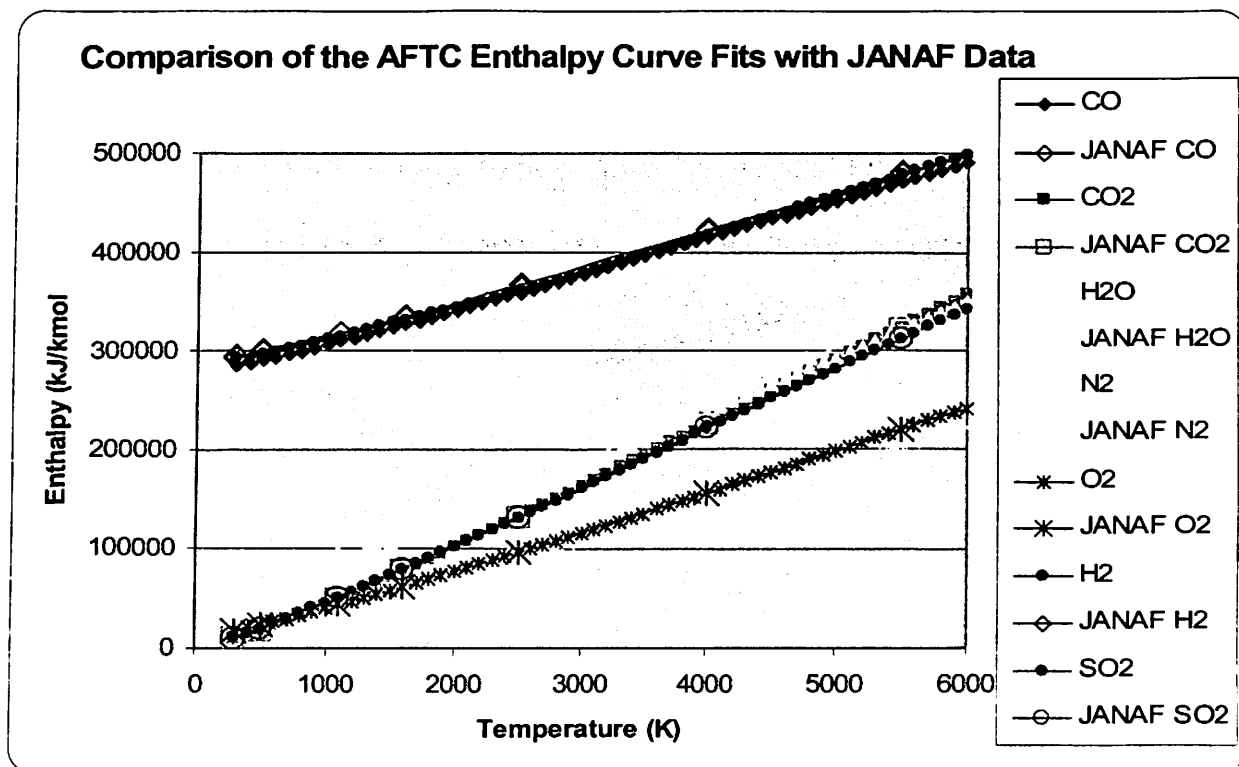
Finally, the table below gives the percent error for the curve fits across several JANAF data points.

Percent Error of Curve Fit Relative to the JANAF Tables							
Temperature (K)	Low (<1600K) and High (>=1600K) Temperature Enthalpy (kJ/kmol)						
	CO	CO_2	H_2O	N_2	O_2	H_2	SO_2
298	2%	1%	3%	3%	4%	0%	0%
500	3%	0%	4%	1%	1%	1%	0%
1100	2%	0%	3%	0%	1%	1%	0%
1600	2%	1%	3%	0%	1%	0%	0%
2500	2%	0%	2%	0%	0%	1%	0%
4000	2%	1%	3%	0%	0%	1%	0%
5500	2%	1%	3%	0%	0%	1%	0%

Appendix D

Fuel Enthalpy Calculations

In order to calculate h_{fuel}, the lower heating value (LHV) of the fuel must be known. A variety of sources were used to find the LHV. However, not all the sources provided the data needed in the required form. Many sources gave the high heating value (HHV). As such, the enthalpy of vaporization for all the water in the products had to be deducted from the HHV. The number of moles of H_2O in a completely combusting system is equal to half the number of atoms of hydrogen in one mole of fuel. Therefore, the LHV is:

$$LHV = HHV - \frac{y}{2}h_{fg_{H_2O}}, \text{ where } h_{fg_{H_2O}} = 44.004 \, MJ\Big/ kg - mol \, H_2O$$

The following spreadsheet was setup to calculate the new LHV for several fuels.

Fuel	n_H in fuel	HHV (MJ/kg fuel)	MWfuel (kg fuel/kmol)	hfg$_{H2O}$ (MJ/kmol H2O)	LHV (MJ/kg fuel)
hydrogen	2	141.6	2.02	44.004	119.771
ammonia	3	22.5	17.03	44.004	18.624
methane	4	55.5	16.04	44.004	50.014
propane	8	50.3	44.10	44.004	46.308
octane	18	47.9	114.23	44.004	44.433
pentadecane	32	47.3	212.42	44.004	43.985
acetylene	2	49.9	26.04	44.004	48.210
naphthalene	8	40.3	128.17	44.004	38.927
methanol	4	22.7	32.04	44.004	19.953

Furthermore, the wood and coal chemical formulas were given based on an "ultimate" analysis, meaning a mass based formulation. These had to be converted to a molar basis. This was done by converting each mass of atoms in the fuel to a molar quantity. Then, with the fuel divided into molar amounts, each quantity was normalized by the total number in the fuel. In this way, the sum of the atoms in the fuel formula equals one.

Appendix E

Fuel Listing

	Composite Fuel Components			Mole Number of Individual Fuel Components					LHV	
Fuel Category	Component Fuel	Molar Perct. Of Composite Fuel	Fuel (gas phase unless otherwise noted)	C	H	O	N	S	(MJ/kg)	
PARAFFINS (C_xH_{2x+2})	1		methane	1	4				50.0471	a
(ALKANES)	2		ethane	2	6				47.5187	a
	3		propane	3	8				46.3865	a
	4		butane	4	10				45.7713	a
	5		pentane	5	12				45.3840	a
	6		hexane (g)	6	14				45.1338	a
	7		hexane (l)	6	14				44.76	e
	8		heptane (g)	7	16				44.9549	a
	9		heptane (l)	7	16				44.59	e
	10		octane (g)	8	18				44.8200	a
	11		octane (l)	8	18				44.43	b
	12		nonane	9	20				44.7149	a
	13		decane (g)	10	22				44.6302	a
	14		decane (l)	10	22				44.27	e
	15		undecane	11	24				44.5339	a
	16		dodecane (g)	12	26				44.467	c
	17		dodecane (l)	12	26				44.14	e
	18		tetradecane (l)	14	30				44.05	e
	19		pentadecane (l)	15	32				43.99	b
	20		hexadecane (l) (cetane)	16	34				43.98	e
ISOPARAFFINS (C_xH_{2x+2})	21		3-methylpentane (l)	6	14				44.73	e
	22		neohexane (l)	6	14				44.59	e
	23		isooctane (l)	8	18				44.35	b
	24		2,3,4-trimethylpentane (l)	8	18				44.41	e
	25		2,2,4,6,8,8-heptamethylnonane	16	34				44.48	e
NAPHTHENES (C_xH_{2x})	26		cyclopentane	5	10				44.2255	a
(CYCLANES)	27		cyclohexane (g)	6	12				43.8634	a
	28		cyclohexane (l)	6	12				43.47	e
	29		methylcyclopentane (l)	6	12				43.68	e
(MISC. NAPHTHENES)	30		tetracyclododecane (l)	12	18				35.38	e
	31		isopropyl bicyclohexyl (l)	15	28				42.71	e
OLEFINS (C_xH_{2x})	32		ethylene	2	4				47.1962	a
(ALKENES)	33		propene	3	6				45.8130	a
	34		1-butene	4	8				45.3485	a
	35		1-pentene	5	10				45.0291	a
	36		1-hexene (g)	6	12				44.8320	a
	37		1-hexene (l)	6	12				44.47	e
	38		1-heptene	7	14				44.6943	a
	39		1-octene (g)	8	16				44.5880	a
	40		1-octene (l)	8	16				44.22	e
	41		2,2,4-trimethyl-2-pentene	8	16				44.00	e
	42		1-nonene	9	18				44.5070	a
	43		1-decene	10	20				44.4419	a
	44		1-undecene	11	22				44.3886	a
	45		1-dodecene	12	24				44.3445	a
	46		eicosane	20	40				44.20	b
ACETYLENES (C_xH_{2x-2})	47		acetylene	2	2				48.2578	a
(ALKYNES)	48		propyne	3	4				46.1999	a
	49		1-butyne	4	6				45.6161	a
	50		1-pentyne	5	8				45.2371	a
	51		1-hexyne	6	10				45.0002	a
	52		cyclohexene (l)	6	10				43.02	e
	53		1-heptyne	7	12				44.8333	a
	54		1-octyne	8	14				44.7093	a
	55		1-nonyne	9	16				44.6129	a
	56		1-decyne	10	18				44.5364	a
AROMATICS	57		benzene (g)	6	6				40.6054	a
	58		benzene (l)	6	6				40.14	b
	59		toluene (g)	7	8				40.9666	a
	60		toluene (l)	7	8				40.55	e
	61		xylene (avg) (g)	8	10				41.2757	a
	62		ethylbenzene (l)	8	10				40.95	e
	63		p-xylene (l)	8	10				40.84	e
	64		styrene (l)	8	8				41.63	e
	65		napthalene (g)	10	8				39.4545	a
	66		napthalene (s)	10	8				38.86	b
	67		sec-butylbenzene (l)	10	14				41.55	e
	68		tetralin (l)	10	12				40.50	e
	69		1-methylnaphthalene (l)	11	10				39.33	e

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				C	H	O	N	S		
ALIPHATIC ALCOHOLS	70		methanol (g)	1	4	1			21.1114	a
(C_xH_{2x},OH)	71		methanol (l)	1	4	1			19.91	b
	72		ethanol (g)	2	6	1			27.7427	a
	73		ethanol (l)	2	6	1			25.82	b
	74		propanol	3	8	1			31.5036	a
MISCELLANEOUS	75		hydrogen (g)		2				120.0338	a
	76		graphite (s)	1					32.7873	a
	77		carbon monoxide	1		1			10.1029	a
	78		cyanogen	2			2		21.06	b
	79		ammonia		3		1		18.61	b
	80		gasoline (l)	7	17				44.51	b
	81		diesel (l)	14.4	24.9				42.94	b
	82		nitromethane (l)	1	3	2	1		10.54	b
	83		good coal (s)	176	144	8	3		31.57	b
	84									
	85									
	86									
	87									
	88									
	89									
	90									
	91									
	92									
	93									
	94									
	95									
	96									
	97									
	98									
	99									
	100									

	Composite Fuel Components									
Fuel Category	Component Fuel	Molar Perct. Of Composite Fuel	Fuel (gas phase unless otherwise noted)	C	H	O	N	S	LHV (MJ/kg)	
SOFTWOODS	101		white cedar (s)	0.18	0.57	0.25			17.69	d
	102		douglas fir (s)	0.20	0.57	0.23			19.17	d
	103		pitch pine (s)	0.21	0.61	0.17			24.08	d
	104		white pine (s)	0.20	0.56	0.24			18.90	d
	105		yellow pine (s)	0.19	0.60	0.21			20.27	d
HARDWOODS	106		white ash (s)	0.18	0.59	0.23			18.72	d
	107		white birch (s)	0.19	0.57	0.24			18.23	d
	108		maple (s)	0.20	0.55	0.24			18.17	d
	109		black oak (s)	0.19	0.55	0.26			17.26	d
	110		red oak (s)	0.18	0.58	0.24			18.29	d
	111		white oak (s)	0.19	0.58	0.24			18.56	d
COALS	112		meta-anthracite (s)	0.90	0.07	0.03			31.76	e
	113		anthracite (s)	0.72	0.26	0.02	0.01		34.20	e
	114		semianthracite (s)	0.64	0.33	0.01	0.01	0.01	35.01	e
	115		low-volatile bituminous (s)	0.61	0.37	0.01	0.01		35.46	e
	116		medium-volatile bituminous	0.57	0.40	0.02	0.01		35.09	e
	117		high-volatile A bituminous (	0.53	0.43	0.03	0.01		34.04	e
	118		high-volatile B bituminous (	0.52	0.42	0.04	0.01	0.01	32.41	e
	119		high-volatile C bituminous (	0.51	0.43	0.05	0.01	0.01	31.85	e
	120		subbituminous A (s)	0.50	0.41	0.08	0.01		29.98	e
	121		subbituminous B (s)	0.46	0.45	0.09	0.01		29.09	e
	122		subbituminous C (s)	0.50	0.40	0.10	0.01		28.10	e
	123		lignite (s)	0.48	0.40	0.11	0.01		27.33	e

References:	
a:	Goodger, E. M., Combustion Calculations, Theory, worked examples, and problems, MacMillian Press LTD, London, 1977
b:	Ferguson, Colin R. and Kirkpatrick, Allan T., Internal Combustion Engines, John Wiley & Sons, New York, 2001
c:	Turns, An Introduction to Combustion, Concepts and Applications, 2nd Ed., McGraw-Hill, Boston, 2000
d:	Strehlow, Roger A., Combstion Fundamentals, McGrawHill, New York, 1984
e:	Bartok, William, and Sarofim, Adel F., Fossil Fuel Combustion: A Source Book, John Wiley & Sons, New York, 1989

Appendix F

User's Guide

In order to create a user-friendly computer program, it was decided to simply incorporate the primary Excel spreadsheet into the user interface. Both program variants run similarly. On the spreadsheet, in the upper-left corner of the page are brief instructions for using AFTC. Below this field are two large buttons, a "run" button and a "clear results" button. Obviously, the run button initiates the computer code. The program will read in all the user supplied fuel data. Then, all other values required by the computer will be calculated, for example, the molecular weights. Next, the fuel is checked against the given oxidizer and the desired results are calculated. The clear results button deletes the content of every cell that is filled with text or by a number when AFTC is run. Both programs use the same input field for the oxidizer as well. An image of this field is supplied below:

"Air"	in form $m(O_2+fN_2+gCO_2)+hH_2O$				Fuel Inlet Temp (K)	Air Inlet Temp (K)	Combustor Pressure (atm)
	Mole Number of Oxidizer Components						
Oxidizer Component	$\phi = m_s/m$	O_2 vol%	g	h			
	1	21	-----	-----	298	298	1

Along the bottom row, the user can simply enter the desired equivalence ratio and oxygen volume percentage in the "air". The grayed out fields are placeholders for future development that will allow the inclusion of carbon dioxide and water in the reactants. In addition, the fuel and air inlet temperatures, as well as the constant pressure in the combustor can be specified. By using Excel, these values are preserved for subsequent program runs with no extra effort from the user.

However, the two programs handle the fuel in slightly different ways. Using a large listing similar to that in Appendix E, the AFTC-Composite program calculates an equivalent composite fuel's physical properties. The molar percentage of each fuel is

supplied by the user in the third column. If that fuel were not in the mixture, the cell is left blank. In this way, the fuel listing can be maintained through a sequence of program runs without having to change the master fuel list. To the right, the fuel's name; carbon, hydrogen, oxygen, nitrogen, and sulfur numbers; and lower heating value are listed. The molecular weight is calculated by the program. For example, if a mixture of equal parts methane and propane were to be burned, the top of the input field would be:

	Composite Fuel Components			Mole Number of Individual Fuel Components					LHV (MJ/kg fuel)
Fuel Category	Fule Number		Fuel (gas phase unless otherwise noted)	C	H	O	N	S	
PARAFFINS (C_xH_{2x+2})	1	50	methane	1	4				50.0471
(ALKANES)	2		ethane	2	6				47.5187
	3	50	propane	3	8				46.3865

where only the first three fuels are shown. A listing of upto 200 fuels would reside in the spreadsheet. The results of the composite fuel program are then displayed in a series of fields across the spreadsheet, according to the specified inlet temperatures and oxygen volume percentages.

The fuel input field of the AFTC-mulifiuel varies with AFTC-composite in that the third column, "Molar Percent. of Composite Fuel", is completely empty. It is not necessary as the program runs through each fuel in the listing, in turn. Except for that previously discussed, the multifuel program is identical to the composite program in appearance. Instead of brief clusters of results spread across the page however, AFTC-multifuel arranges its data in several columns:

With Dissociation

Fuel Category	Fuel Name	Carbon Number	Adiabatic Flame Temperature (K)	
PARAFFINS (CxH2x+2)	methane	1	2248	
(ALKANES)	ethane	2	2283	
	propane	3	2291	
	butane	4	2294	
	pentane	5	2296	
	hexane (g)	6	2297	
	hexane (l)	6	2286	
	heptane (g)	7	2298	
	heptane (l)	7	2288	
	octane (g)	8	2299	
	octane (l)	8	2288	
	nonane	9	2300	
	decane (g)	10	2301	
	decane (l)	10	2290	
	undecane	11	2300	
	dodecane (g)	12	2300	
	dodecane (l)	12	2290	
	tetradecane (l)	14	2291	
	pentadecane (l)	15	2291	
	hexadecane (l) (cetane)	16	2291	
ISOPARAFFINS (CxH2x+2)	3-methylpentane (l)	6	2285	

In this example, the oxidizer was standard dry air. The fuel category and name are repeated with each set of results for conviencence. Then the corresponding carbon number and adiabatic flame temperatures are given. Minimal coding effort would be required to display results for any other quantity found by AFTC. Finally, three more sets of data like the above example are calculated, for all fuels listed, for the four cases of dissociation and no dissociation, each in either a user supplied "air" and pure oxygen.

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