Thermal Field Characteristics with Alternative Fuels in Advanced Power Generation

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Abstract

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

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

1. Introduction

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

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

None of these texts give general computerized methods for finding the adiabatic flame temperature and product species amounts, including some degree of dissociation. Only advanced research reports (for example, Gordon and McBride (1971)) give very general computerized methods with a significant sophistication given to the dissociation aspects of the calculation. Some combustion-oriented texts do include computerized calculations of flame temperature (Borman and Ragland (1998) and Turns (2001)) with the inclusion of computer codes, see Turns (2001). None of them present easily computerizable flame temperature and species calculation methodologies, that can be used by the practicing applied combustion engineer. The present objective is to present a useful Exce/VBA code that permits easily a wide range of calculations to be accomplished and graphed easily by the practical man.

A straightforward computer code has been developed and is now described which calculates the adiabatic flame temperature and product species amounts for general CHONS fuels. The program is named Adiabatic Flame Temperature Calculation (AFTC). It is useful for calculations within in a computational fluid dynamics reacting flow computation, and it is readily incorporated into undergraduate

and graduate course studies. It is based on the methods of Goodger (1977) and Campbell (1979). The theoretical background and computational algorithms used in its development are presented. The parameters used are: fuel type, equivalence ratio, reactant temperatures and pressure, type of oxidant and air composition, and inclusion of dissociation effects. This work builds on previous papers, Lilley (2004) and Olinger and Lilley (2004a and b, and 2005a). Results are given for a range of input parameters so as to illustrate the versatility of the computer program. Associated results applicable to the new technology of high temperature air combustion are given in an associated paper; see Olinger and Lilley (2005b).

2. Computational Method

In all these HiTAC technologies, it is important to know the flame temperature and corresponding product composition. However, experimentation to determine this is very delicate, costly, and time consuming. For this reason, theoretical calculations are preferred. The very-general fuel is specified by way of its C-H-O-N-S content and additional water content and the "air" by way of the volume percent of oxygen, and the other component of "air" (nitrogen and/or carbon dioxide), each specified by the user. The temperature of each inlet (fuel and "air") is specified by the user, so is the equivalence ratio. Then, results of adiabatic flame temperature are calculated along with the equilibrium product species both with and without dissociation. The author has developed this computer code, written in Excel/VBA, that can make these computations quickly and easily, with a wide variety of easily incorporated complexities, specifically useful for the HiTAC technology and more general pure and applied combustion applications, see Lilley (Ref. 4). The standard expression for general fuel-air combustion is:

$$C_x H_y O_z N_u S_v + m(O_2 + f N_2 + g\,CO_2) + h\,H_2O \rightarrow$$

$$n_1 CO + n_2 CO_2 + n_3 H_2O + n_4 N_2 + n_5 O_2 + n_6 H_2 + n_7 SO_2$$

The right hand side represents the major combustion product species. A half-interval search technique is used to determine the temperature, where at each temperature the right hand side species amounts are either known (the no dissociation assumption) or a half-interval search technique is used to determine the species (the with dissociation case).

Dissociation reactions absorb thermal energy, thus lowering the product flame temperature. With combustion at relatively cool temperatures, dissociation is minimal and from the temperature and species point of view, the major dissociations are with carbon dioxide and water vapor dissociating. One of the simplest and most effective assumptions about dissociation is that 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. Additionally, but to a lesser degree, more complex dissociated product species may occur, including O, H, OH, and NO. The degree of dissociation is dependent on both the combustion pressure and temperature, and is such that the molar (volume) fractions obey the laws of mass action.

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

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

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

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. Temperature and products are calculated for each fuel in turn, allowing automatic, fast generation of eight graphs and useful tables. These permit immediate comparison of different fuels and

properties, such as how the adiabatic flame temperature varies with the carbon number of a fuel, equivalence ratio, inlet reactant temperatures, etc.

3. Results and Discussion

3.1 Comparison with Other Methods

Other methods exist that may offer a more direct solution to the above equations, but at the cost of guaranteed convergence, Campbell (1979). One such method for solving the flame temperature and product composition is to use a Newton-Raphson iteration procedure. This is the method used in both the well-known programs by Turns (2001) and Gordon-McBride (1971). It is also implemented in Ferguson and Kirkpatrick (2001). In addition to the dissociated species accounted for in AFTC, these programs also account for H, NO, O, OH, and N. Goodger (1977) also gives temperature predictions. The present code has been run for a variety of situations and compared very favorably, typically less than a one percent difference in temperature. The results for Turns were obtained by running the program. Results for Gordon-McBride were cited in Glassman (1987). Results for Goodger (1977) and Ferguson and Kirkpatrick (2001) are from their respective books. Table 1 displays the adiabatic flame temperature found by each program. Table 2 then recalculates the results of Table 1 to give each program's percent difference in temperature, relative to the present AFTC calculations.

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

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

Comparison of Adiabatic Flame Temperatures (K)						
Fuel	**Formula**	**AFTC**	**Goodger**	**Turns**	**F&K**	**G&M**
Methane	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 2. Percent differences of the dissociated stoichiometric adiabatic flame temperature (K) as predicted by AFTC, Goodger (1977), Turns (2001), Ferguson and Kirkpatrick (2001), and Gordon and McBride (Glassman, 1987) in dry standard air.

Percent Differences in Adiabatic Flame Temperature Calculations						
Fuel	**Formula**	**AFTC**	**Goodger**	**Turns**	**F&K**	**G &M**
Methane	CH_4	0	-0.03	-0.97	-0.92	-1.68
Propane	C_3H_8	0	0.67	-0.30	-0.26	-
Heptane	C_7H_{16}	0	0.76	-0.30	-	0.40
Acetylene	C_2H_2	0	0.99	-0.73	-0.69	-
Methanol	CH_3OH	0	0.63	-0.35	-	-
Hydrogen	H_2	0	1.05	-1.52	-1.47	-0.77
Carbon Monoxide	CO	0	1.46	0.78	-	1.50
Cyanogen	C_2N_2	0	-	0.21	0.29	-

3.2 Comparison of General HC Fuels

After the comparison with other computer programs, AFTC was run for a variety of different fuels and equivalence ratios, the results of which are displayed at the end of this paper. For example, many fuels, grouped into acetylenes, paraffins, and olefins, are calculated for stoichiometric combustion. These results are given in Figure 1. The adiabatic flame temperature is graphed against the carbon number of the fuel. Notice all the curves, each representing a different class of fuels, converge to one temperature as the carbon number increases. This is justification for the common practice in industry of modeling complex fuels as composites of simpler fuels.

After these results were displayed, the equivalence ratio was changed to fuel lean and fuel rich conditions. From Figures 2 and 3, one finds the temperatures are highest for nondissociated combustion. As the equivalence ratio shifts from unity, the temperature decreases.

3.3 Comparison of CHON Fuels

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

4. Conclusions

A calculation procedure in Excel/VBA has been developed that quickly calculates the combustion product composition and temperature. This procedure has been applied to the combustion of a range of fuel compositions related to alternative fuels and processing of municipal solid waste. 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. Results show the accuracy, robustness and versatility of the code, and its ease of applicability to realistic combustion situations. Current application is to a vast range of additional reaction features.

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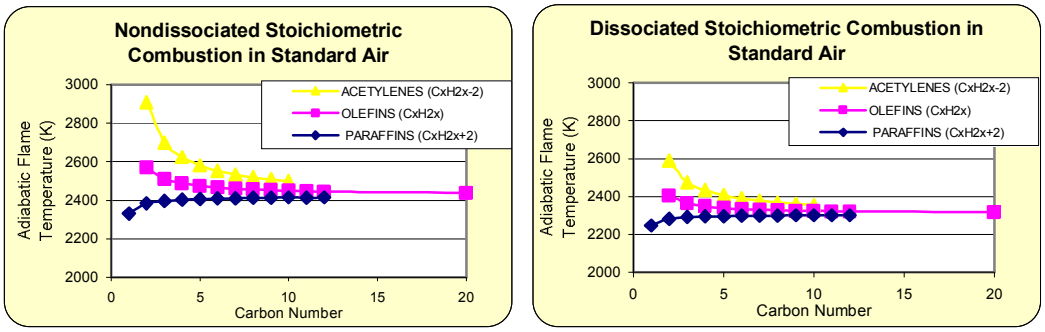

Figure 1. Stoichiometric Adiabatic Flame Temperature as a Function of the Fuel Carbon Number.

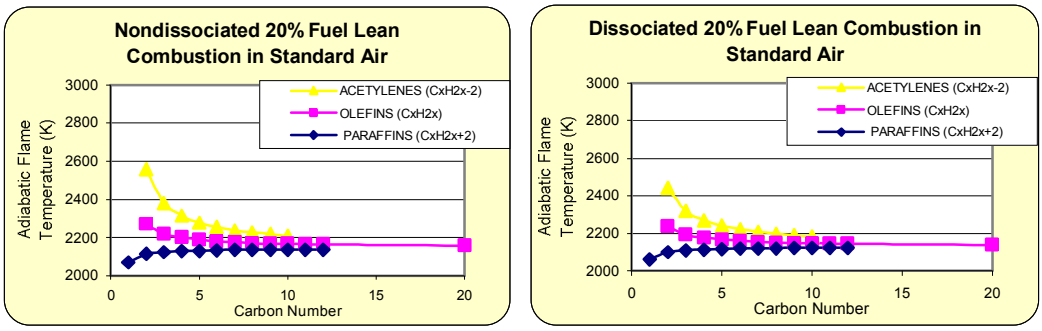

Figure 2. 20% Fuel Lean Adiabatic Flame Temperature as a Function of the Fuel Carbon Number.

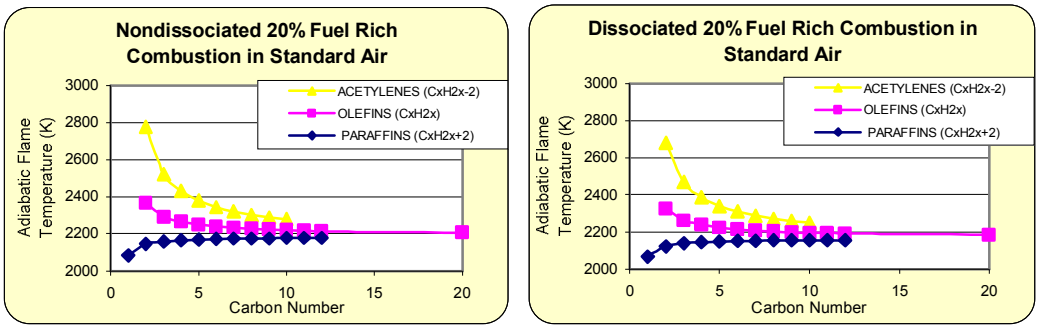

Figure 3. 20% Fuel Rich Adiabatic Flame Temperature as a Function of the Fuel Carbon Number.

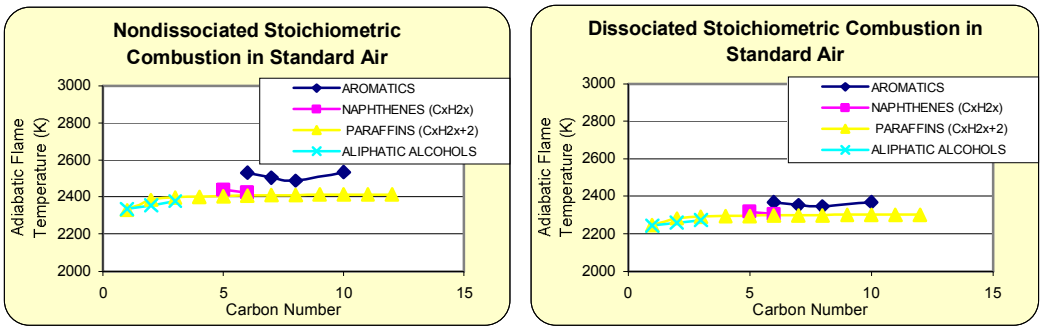

Figure 4. Stoichiometric Adiabatic Flame Temperature as a Function of the Fuel Carbon Number.

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Author Biography

Dr. David G. Lilley is a Professor in the School of Mechanical and Aerospace Engineering, Oklahoma State University, U.S.A., with expertise in combustion aerodynamics. His active consulting practice Lilley & Associates is primarily concerned with litigation emphasizing fires, combustion, fuels, aerodynamics, fluid dynamics, heat transfer, fuel sprays, and computer simulation. He was born in England and obtained his education at Sheffield University, from which he received the Bachelor and Master degrees in Mathematics in 1966 and 1967, and the Ph.D. degree in Engineering in 1970. The "higher doctorate" D.Sc. degree was awarded in 1991 by Sheffield University for many years of successful research, publication of high quality original research work, international recognition, and standing as an authority in the field Combustion Aerodynamics. The "Energy Systems Award" was given in 1992 by AIAA for distinguished contribution as a teacher, researcher and consultant in the areas of swirl flows in combustors and furnaces, mathematical modeling, fuels and fires. In 1993 he was elected to the grade of Fellow of the AIAA - an honor bestowed upon people of distinction who have made notable and valuable contributions to the arts, sciences, or technology of aeronautics or astronautics. In 2000 he was elected to the grade of Fellow of the ASME and awarded the "George Westinghouse Gold Medal" for notable contributions to the Power Field of Mechanical Engineering, specifically for distinguished contributions as a teacher, researcher and consultant in power engineering, including the publication of quality scholarly papers and studies on safety, energy efficiency and environmentally compliant power systems. In 2008, he was awarded the ASME "Holley Medal" for exemplary contributions to the development of science and engineering of fires, their growth and fire accident prediction and practical aspects of fire investigation that has resulted in greater public safety and reliability from a wide range of fuels use and application.