

A Theoretical Analysis for Modeling and Prediction of the Jet Engine Emissions

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Abstract—This paper is to formulate a mathematical model to predict the amounts of the emissions produced from the combustion process of the gas turbine unit of the jet engine. These emissions have bad impacts on the environment if they are out of standards, which cause real threats to all type of life on the earth. The amounts of the emissions from the gas turbine engine are functions to many operational and design factors. In landing-takeoff (LTO) these amounts are not the same as in taxi or cruise of the plane using jet engines, because of the difference in the activity period during these operating modes. These emissions can be affected by several physical and chemical variables, such as fuel type, fuel to air ratio or equivalence ratio, flame temperature, combustion pressure, in addition to some inlet conditions such as ambient temperature and air humidity. To study the influence of these variables on the amounts of these emissions during the combustion process in the gas turbine unit, a computer program has been developed by using the visual basic 6 software. Here, the analysis of the combustion process is carried out by considering it as a chemical reaction with shifting equilibrium to find the products of the combustion of the octane fuel, at different equivalence ratios, compressor pressure ratios (CPR) and combustion temperatures. The results obtained have shown that there is noticeable influence of the equivalence ratio, CPR, and the combustion temperature on the amounts of the main emissions which are considered pollutants, such as CO, CO₂ and NO.

Keywords—Mathematical model, gas turbine unit, equivalence ratio, emissions, shifting equilibrium.

I. INTRODUCTION

MANY of today's applications require a theoretical and actual analysis of their processes, especially combustion process which has been involved in many applications in our life. The combustion process consists of the oxidation of constituents in the fuel that are capable of being oxidized and can therefore be represented by a chemical equation. During a combustion process, the mass of each element remains the same. Thus, writing chemical equations and solving problems concerning quantities of the various constituents basically involve the conservation of mass of each element [1]. When a chemical reaction occurs, the bonds within molecules of the reactants are broken, and atoms and electrons rearrange to form products. In combustion reactions, rapid oxidation of combustible elements of the fuel results in energy release as combustion products are formed. The three major combustible chemical elements in most common fuels are carbon, hydrogen, and sulfur. Sulfur is usually a relatively

unimportant contributor to the energy released, but it can be a significant cause of pollution and corrosion problems. Combustion process is considered complete when all the carbon present in the fuel is burned to carbon dioxide, all the hydrogen is burned to water, all the sulfur is burned to sulfur dioxide, and all other combustible elements are fully oxidized. When these conditions are not fulfilled, combustion is incomplete. Combustion is the result of a series of very complicated and rapid chemical reactions, and the products formed depend on many factors. When fuel is burned in the cylinder of an internal combustion engine, the products of the reaction vary with the temperature and pressure in the cylinder. In combustion equipment of all kinds, the degree of mixing of the fuel and air is a controlling factor in the reactions that occur once the fuel and air mixture is ignited. Although the amount of air supplied in an actual combustion process may exceed the theoretical amount, it is not uncommon for some carbon monoxide and unburned oxygen to appear in the products. This can be due to incomplete mixing, insufficient time for complete combustion, and other factors. When the amount of air supplied is less than the theoretical amount of air, the products may include both CO₂ and CO, and there also may be unburned fuel in the products [2]. These products are considered one of the main sources of air pollutants. Air pollutants may be classified into two broad categories: (1) natural and (2) human-made. Also they could be classified according to the origin, where they could be primary or secondary. In the primary, the pollutants are emitted to the atmosphere from the process, while in the secondary, they are formed in the atmosphere as a result of a chemical reaction. Also they may be classified as to the state of matter, which could be gaseous such as nitrogen oxide, carbon monoxide, etc., and particulate such as dusts, smokes, droplets, etc. [3].

Potential air pollutants are not only toxic in many cases, but they can travel over great distances, thereby contaminating areas far away from the sources of emissions. There are two environments that are of concern, once chemicals are emitted to the surroundings: The general atmosphere, and the work space. In the first environment, we are concerned with the potential health risks that chemicals pose to the public, as well as possible impacts on the ecology. In the latter case, we are concerned with indoor air quality and its possible adverse impacts on the health and safety of the workforce. In both cases, the health dangers may be either acute or long-term chronic health risks [4].

Seinfeld [5] indicates four principle effects of air pollutants

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in the troposphere:

1. Altered properties of the atmosphere and precipitation.
2. Harm to vegetation.
3. Soiling and deterioration of materials.
4. Potential increase of morbidity (sickness) and mortality in humans.

One of the results of the pollutants is the greenhouse gases which may alter local climates. Also, acid rains, produced from SO_x and NO_x emissions, affect lakes and susceptible soils [6]-[8]. On the health side, it is well known that the pollutants can aggravate pre-existing respiratory ailments. Secondary pollutants in photochemical smogs cause eye irritation. These pollutants -ozone, organic nitrates, oxygenated hydrocarbons, and photochemical aerosol- are formed primarily by the reactions among nitric oxides and various hydrocarbons. Also, carbon-based particles may contain adsorbed carcinogens. In addition to the concerns enumerated here, all of which are related to pollutants in the troposphere layer and emission of NO_x into the stratosphere by high-speed civil transport (HSCT) aircraft are also of interest. Concern here is about the catalytic destruction of stratospheric ozone by NO following the reaction mechanism

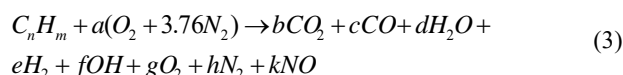


Noted here that O_3 is destroyed in the first reaction by NO, while NO is regenerated in the second reaction to enter again into the O_3 -destruction step. Removal of O_3 from the stratosphere allows more harmful ultraviolet solar radiation to penetrate to Earth's surface [9].

Recent investigations have introduced a lot of new and exciting research into increasing the efficiency of combustion systems of the power plants. New ways of combining power cycles to increase greater percent excess air and hotter reaction temperatures have increased the thermal efficiency to around 60%, and the percentage is continually being increased with new researches. In the combined-cycle power plant, the flue gases exhausted from the gas turbine unit are directed to a heat exchanger which is working as a boiler in the steam unit, and is called a heat-recovery steam generator (HRSG). Upon this fact about the danger of the combustion products on the life of the human beings this study is carried out to formulate and simulate the combustion process of the hydrocarbon fuels used in gas turbine engines. This is done by taking the dissociation process into account during the reaction with a shifting equilibrium of the species of the product. Here, a software has been developed to find the amounts of the species with the emission indices of the main pollutants. In this software the inputs can be varied according to the selected type of the fuel which could be octane or any other to obtain the required results at the browse of this software.

II. MATHEMATICAL MODEL

In high-temperature combustion processes, the products of combustion are not a simple mixture of ideal products, as may be suggested by the simple atom-balance used to determine stoichiometry. Rather, the major species such as CO_2 , H_2O , O_2 , and N_2 dissociate, producing a host of minor species, such as H_2 , OH, CO, and NO, and possibly more others like O, H, and N. Here, we have to find the mole fractions of all product species at a given temperature and pressure, based on the identity that the number of the main elements introduced in the chemical reaction stays constant, regardless of how they are combined in the various species. According to this real assumption, the combustion of an arbitrary hydrocarbon with excess air can be represented as



where

$$a = (1+x)\left(n + \frac{m}{4}\right) = \left(\frac{1}{\phi}\right)\left(n + \frac{m}{4}\right) \quad (4)$$

ϕ is the equivalence ratio (ER) and it is a function of excess air percentage commonly used to indicate quantitatively whether a fuel-oxidizer mixture is rich, lean, or stoichiometric. For rich mixture $\phi > 1$, and for lean $\phi < 1$. The other constants in (4) are the number of moles of the product species, which are unknown values, and have to be determined by formulating eight equations equal to the number of these unknown values. In this case, three equations could be obtained from the mole ratios of the main atoms. Four other equations can be determined from the equilibrium constants during dissociation, and the final one comes from the fact that the summation of the mole fractions of the product species is unity. These equations are as:

$$\text{RCH} = \frac{b+c}{2d+f+2e} = \frac{N_c}{N_H} \quad (5)$$

where RCH is the ratio of carbon atoms to hydrogen atoms in the reactants, this ratio could be written in terms of mole fractions of the same species instead of number of moles, this ratio becomes:

$$\text{RCH} = \frac{\chi_{\text{CO}_2} + \chi_{\text{CO}}}{2\chi_{\text{H}_2\text{O}} + \chi_{\text{OH}} + 2\chi_{\text{H}_2}} \quad (6)$$

By similar way we get the nitrogen to oxygen ratio (RNO) and the oxygen to hydrogen ratio (ROH) as follows:

$$\text{RNO} = \frac{\chi_{\text{NO}} + 2\chi_{\text{N}_2}}{2\chi_{\text{CO}_2} + \chi_{\text{H}_2\text{O}} + \chi_{\text{CO}} + \chi_{\text{OH}} + \chi_{\text{NO}} + 2\chi_{\text{O}_2}} = \frac{N_N}{N_O} \quad (7)$$

also we have

$$ROH = \frac{2\chi_{CO_2} + \chi_{H_2O} + \chi_{CO} + \chi_{OH} + \chi_{NO} + 2\chi_{O_2}}{2\chi_{H_2O} + \chi_{OH} + 2\chi_{H_2}} = \frac{N_O}{N_H} \quad (8)$$

The summation of these mole fractions is unity, thus

$$\chi_{CO_2} + \chi_{CO} + \chi_{H_2O} + \chi_{H_2} + \chi_{OH} + \chi_{O_2} + \chi_{N_2} + \chi_{NO} = 1.0 \quad (9)$$

The available information concerning equilibrium state in the current combustion process is of the following forms:



From these four equations we get four equilibrium constants as a function of pressure ratios of each constituent, which can be replaced by mole fractions as:

$$\chi_{CO_2} = K_{p_{CO_2}} \cdot \chi_{CO} \cdot \chi_{O_2}^{0.5} \cdot P_c^{0.5} \quad (14)$$

$$\chi_{H_2O} = K_{p_{H_2O}} \cdot \chi_{H_2} \cdot \chi_{O_2}^{0.5} \cdot P_c^{0.5} \quad (15)$$

$$\chi_{OH} = K_{p_{OH}} \cdot \chi_{H_2}^{0.5} \cdot \chi_{O_2}^{0.5} \quad (16)$$

$$\chi_{NO} = K_{p_{NO}} \cdot \chi_{N_2}^{0.5} \cdot \chi_{O_2}^{0.5} \quad (17)$$

In these equations the equilibrium constants can be calculated at a given temperature from the standard-state Gibbs function change ΔG_T° , as:

$$K_p = \exp(-\Delta G_T^\circ / R_u T) \quad (18)$$

Here the Gibbs function change is determined for each equilibrium reaction from its definition which is given by [10]:

$$\Delta G_T^\circ = \sum_p n_j \bar{g}_T^\circ - \sum_r n_i \bar{g}_T^\circ \quad (19)$$

where

$$\bar{g}_T^\circ = R_u T \left[a_1 (1 - \ln T) - \frac{a_2}{2} T - \frac{a_3}{6} T^2 - \frac{a_4}{12} T^3 - \frac{a_5}{20} T^4 + \frac{a_6}{T} - a_7 \right] \quad (20)$$

The constants a_1, a_2, \dots, a_7 are the temperature coefficients according to the types of gases in the products and reactants of the equilibrium reaction.

Equation (18) shows that the equilibrium constant K_p is

dependent on ΔG_T° , which gives a qualitative indication of whether a particular reaction can go strongly to completion, tending to favor products, or can go weakly, tending to favor reactants at equilibrium. In the first case, the Gibbs function ΔG_T° will be negative value, while in the second case the value of this function will be positive [9].

Now, to find the mole fractions given in the above equations a numerical method, which is iteration, has to be used, because these equations are non-linear and cannot be solved simultaneously. In this case a computer program using visual BASIC code has been developed by starting with initial values of χ_{O_2} & χ_{N_2} as a first estimation, and calculating the others. The correct results being determined by updating the new values each loop and comparing with the known mole ratios, until the differences between the calculated and known values diminish.

After we find the mole fractions of the product species we can determine the emission indices of the main pollutants such as CO and NO. The emission index is particularly useful in that it unambiguously expresses the amount of pollutant formed per mass of fuel, independent of any dilution of the product stream or efficiency of the combustion process.

For the combustion of a hydrocarbon fuel in air, the emission index can be determined from mole fractions of the species of interest, together with those of all of the carbon-containing species as in the following equation:

$$EI_i = \left(\frac{\chi_i}{\chi_{CO} + \chi_{CO_2}} \right) \left(\frac{N_c M_i}{M_f} \right) \quad (21)$$

Physically, the first bracketed term in (21) represents the number of moles of i per mole of carbon originating in the fuel, while the other term provides the necessary conversion of carbon moles to fuel moles and their respective conversion to mass units.

It is next important to determine the rate at which the products will reach equilibrium. The basic mechanism presently used to predict the formation of NO has been developed by Wark and Warner [10] as:

$$(1 - Y)^{C+1} (1 + Y)^{C-1} = e^{-Mt} \quad (22)$$

where

$$Y = [NO]/[NO]_e \quad (23)$$

$$C = \frac{(2.1 \times 10^4) [\chi_{N_2}]^{0.5} e^{-7750/T_c}}{T_c [\chi_{O_2}]^{0.5}} \quad (24)$$

$$M = \frac{(5.4 \times 10^{15}) (P_c)^{0.5} [\chi_{N_2}]^{0.5} e^{-58330/T_c}}{T_c} \quad (25)$$

Fig. 1 The page of the constructed software

From (22) we can determine the formation time of NO at many different values of concentration ratios with respect to equilibrium case, i.e. (23), which is already available from previous equilibrium reactions. Also, it is of interest to determine this time for various temperatures, pressures and equivalence ratios.

III. RESULTS AND DISCUSSION

To check the validity of the above mathematical model, the octane fuel has been used to study the influence of some input variables such as equivalence ratio, combustion temperature and CPR on the amounts of the product species of this fuel. The software constructed in this case can take any relevant values of the input variables, as shown in Fig. 1. By using the page of this software the results obtained are depicted in the following figures. In Fig. 2, the concentration percent of CO₂ produced from the combustion of octane decreases with excess air and with rich fuel, where formation of CO takes place and increases with the equivalence ratio.

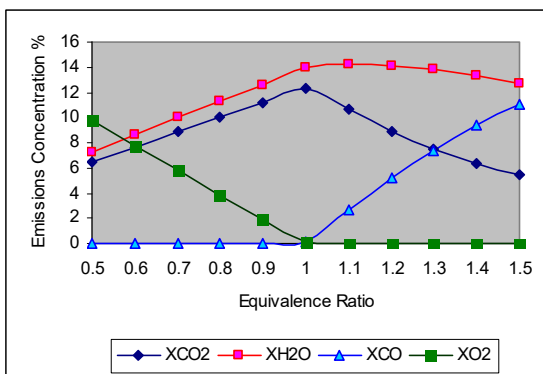
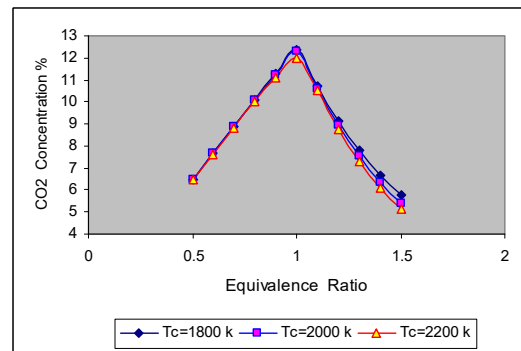


Fig. 2 Emissions concentrations vs ER

For excess air process there is sufficient O₂ to have all the fuel C and H react to form CO₂ and H₂O, while in rich case there is not enough O₂ to complete the reaction.

Fig. 3 CO₂ concentration vs T_c & ER

The other influential parameter on the amounts of the emissions is the combustion temperature, here we notice in Fig. 3 that the amount of CO₂ decreases as the temperature increases to a value close to adiabatic flame temperature of octane. Carbon dioxide is responsible for more than 50% of the man-made greenhouse effect, making it the most important contributor to climate changes in the global average temperature and of the seasonal cycle [12]. The burning of fuels is the main reason for the formation of this gas, and in any case this gas will be produced, even in the ideal reactions such as stoichiometric. To reduce the amount of this pollutant (CO₂), it is advisable to use renewable resources such as solar energy instead of conventional resources such as fossil fuels. In Fig. 4 the emission index of NO goes up with the temperature and with the amount of O₂ due to more dissociation of N₂ at higher temperatures. In this case, NO can be formed through several mechanisms and variations thereof.

Bowman [11] classifies these into the following two categories:

1. The extended Zeldovich (or thermal) mechanism in which O, OH, and N_2 species are at their equilibrium values and N atoms are in steady state.
2. Mechanisms whereby NO is formed more rapidly than predicted by the thermal mechanism above, either by (i) the Fenimore CN and HCN pathways, (ii) the N_2O -intermediate route, or (iii) as a result of super equilibrium concentrations of O, and OH radicals in conjunction with the extended Zeldovich scheme.
3. Fuel nitrogen mechanism, in which fuel-bound nitrogen is converted to NO.

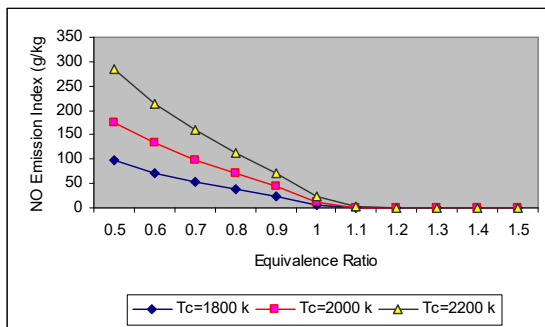


Fig. 4 NO emission index vs T_c & ER

If the levels of NO are lower than their equilibrium values and reverse reactions are unimportant, the NO yield is directly proportional to time. However, in the design of a combustion system, the temperature-versus-time relationship is key to the control of NO emissions, so any alteration of this relationship for the gas flow may compromise the useful operation of the device [9].

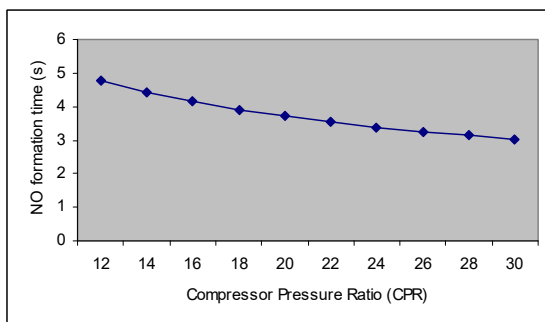


Fig. 5 NO formation time vs. CPR

In gas turbine engines the CPR plays an important rule on the performance of this engine. It is known from previous studies that the output power and the efficiency improved by increasing CPR to a certain value. In the current analysis we notice in Fig. 5 that the formation time of NO goes down with CPR at a certain temperature and equivalence ratio, unfortunately this is not good during high activity periods which required high values of CPR.

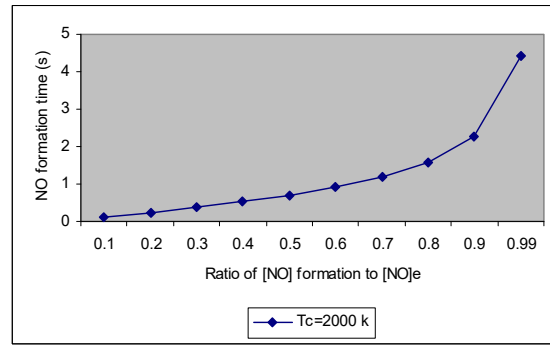


Fig. 6 The historical period of NO formation

While in normal operations at a certain CPR and temperature, the amounts of NO takes long time to be formed as shown in Fig. 6, which gives less concentration of this pollutant in atmosphere.

IV. CONCLUSION

The present investigation is carried out to formulate a mathematical model and construct a software to study the influence of some practical parameters such as combustion temperature, equivalence ratio and CPR on the amounts of emissions produced from burning octane fuel in the gas turbine unit of the jet engines. The code of the program has been written in a general form in which any type of fuel with known numbers of atoms could be used in the analysis to find the product species at specified values of the performance parameters.

From the results obtained we deduce that there is a great influence of the combustion temperature and equivalence ratio on the concentrations of the emissions, in which they are lower at high excess air and high values of combustion temperature. In this case, to effectively stem the greenhouse effect, emissions of CO_2 , must therefore be greatly reduced, with other emissions such as CO and NO.

Other benefits could be obtained from the constructed model is its ability to calculate the amounts of heat energy during combustion, and this will help us to make a compromise between different types of hydrocarbon fuels. In addition of that it could be used to study the combustion process of the hydrogen, which is also expected to play a major role as energy carrier for the renewable energies, mainly solar energy. Also we could find the adiabatic flame temperature of combustion of any other fuel has known formation enthalpy.

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