High Altitude Micro gas turbine power plant investigation of Parametric Analysis using Quantum Chemistry techniques for Alternate fuel optimization.

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Abstract. Non-petroleum-based fuels help in mitigating climate change by reducing the emission. Many studies on the emission characteristics for the alternate fuel dimethyl ether (DME), resulted in a significant reduction in NOx, SOx, and particulate matter. Due to the potential impact of the use of DME, a need for an Alternate fuel powered Micro gas turbine power plant for high altitude flight was investigated. The potential energy of DME reacting with oxygen was calculated in the temperature range 800–1350 K at the total pressure exhibited on combustion chamber similar to that of high altitude flight. Multichannel ab-initio and RRKM calculation were performed on the DME combustion reaction in the presence of air \( C_2H_6O+O_2+N_2 \rightarrow CO_2+H_2O+N_2 \). The computed energy value obtained at low pressure was used to study the thermodynamic cycle of a 6kW micro gas turbine power plant for the use of power generation at high altitude flight system. The resulting energy flow model obtained is significant to understand the system performance and efficiency optimization.

1. Introduction
Combining Turbomachinery with Combustion model has a huge impact in designing a Gas turbine power plant; however, little research exists in this direction. This investigation aims to develop a parametric model to optimize the thermodynamic cycle using quantum chemistry techniques. Many countries in the last decade have dedicated interest to reduce the consumption of fossil fuels for fighting global climate change. This widens the importance of research to reduce energy consumption by increasing the overall efficiency of the power plant [1- 2].

In this research parametric analysis of 6kw micro gas turbine power plant was investigated to generate electrical energy for very high-altitude flights (in the range of 18-22 km). The system consists of a radial compressor, combustion chamber, axial turbine, and generator. The article is divided into two parts, one focuses on thermodynamic cycle optimization for a high-altitude gas turbine using the standard thermodynamic equations while the other part focuses on optimizing the energy of the fuel at the quantum level.

However, to be certain the quantum chemistry techniques, the goal is NOT to provide computation research for understanding combustion properties of DME but to provide an optimization model for designing efficient Micro gas turbine power plant by interconnecting thermodynamic calculation and chemical kinetics.

- Thermodynamic Analysis.
- Quantum chemistry techniques.
Power generating micro gas turbine efficiency relies heavily on ambient climate conditions. At the high altitude, investigation provides valuable insight and research data for optimizing the overall cycle efficiency of a micro gas turbine. Ambient weather condition primarily depends on parameters like Hot climates, High Altitudes, rapid temperature fluctuations, and more importantly humidity. The ambient condition influences the output power generating capabilities. The micro gas turbine power plant is expected to behave differently alternatively to initial design conditions, in particular parameters for instances total power obtained, Specific fuel consumption and the overall efficiency of the power plant. This makes it important to investigate the ambient conditions in the function of Ambient Temperature, Ambient Humidity and Ambient Pressure at the required altitude. To avoid designing of particular geographical location, vast parametric data is considered in the thermodynamic cycle optimization.

At high altitude the density of air is scarce, thus, influences negatively on the output power of the micro gas turbine power plant. The Ambient pressure decreases with increase in altitude causing the insufficient flow to the combustion chamber and requires extra power for the compressor performances. To understand the density of ambient air a mathematical model consisting of ambient temperature, ambient humidity conditions were developed by the data assist from Reference [3-6].

2. Why quantum level analysis is required?

In a micro gas turbine power plant, the output power depends on the mass flow rate of the compressor output and the Turbine inlet temperature; however, the ambient conditions play a vital role on the effects of power plant efficiency. The power of the compressor can increase and decrease in accordance with the ambient conditions. As a result, gas turbine engine designers need to determine the optimum output power ratio gained in compressor work done performed. At high altitudes, oxygen content decreases with every increase in altitude, thus the possibility of inefficient combustion resulting reduces thermal efficiency. In this research, a quantum methodology helps in understanding the combustion of the DME at lower pressures and of the oxygen stagnation environment. The reaction is mainly computed for rate constant during the chemical reaction for combustion, the process at high altitude in order to determine losses while in actual operation. Geometry optimization is the basic component used in modeling molecules. The calculations involved are used to find the coordinates or the positions of the atoms of the molecule where it has the minimum energy and is hence stable.

3. Choice of Fuel

Dimethyl Ether (DME) with the chemical formula $\text{CH}_3\text{O-CH}_3$, exists as an invisible gaseous ether compound under atmospheric conditions (0.1 MPa and 298 K) but it must be condensed to the liquid phase by pressurization above its vapor pressure at 0.5 MPa (5.1 bar or 73 psi) at 25°C to be used as a diesel alternative fuel [18]. The advantage of DME is that it can be produced from any kinds of carbon resources, such as natural gas, coals or biomass gasification through synthesis gas. DME has a high cetane number (55 to 60) which allows to decreases engine knocking and engine noise when compared to engines powered with traditional diesel.[19] Fuels such as natural gas and propane have octane numbers greater than 100 but cetane numbers are lower than 10 which makes them infeasible for perfect use of a diesel cycle engine. As DME has high cetane number allow complete combustion process with less wastage of fuel, particularly at engine start-up or when the cylinder temperatures cool off. [19]

One of the compelling features of DME involves no direct carbon-to-carbon bond that is found in common diesel fuels. Conventional diesel contains no oxygen while DME is an oxygenated fuel and contains about 34.8% oxygen by mass with no carbon-to-carbon bonds. The high cetane number and oxygen content significantly improved the combustion and emission characteristics such as early ignition and low PM and NOx emissions. In the sense, DME deserves for a potential alternative fuel and solution to energy problems even considering environmental importance. [18]. Other important properties of DME when dealing with combustion is mentioned below are as follows: [20]

- Weight base calorific value methane > Propane > DME > methanol
- Gaseous volume calorific volume Propane > DME > methane
• Similar properties to LPG and thus dealing for LPG are easy to apply to DME storage
• Toxic level is similar to that of propane, but DME has neither greenhouse effect nor ozone layer depletion.

4. Methodology
The ultimate research need for any micro gas turbine engine is the improvement in efficiency and performances done through thermodynamic cycle analysis based on the first and second laws of thermodynamics. The current work provides the integration of thermodynamics with chemical kinetics at the quantum level of the hot working fluid. A numerical investigation comparison was performed on a 6 kW micro gas turbine with and without the quantum level parametric analysis. The results show how various design parameters affect the output power and overall efficiency.

Achieving higher thermal efficiencies for micro gas turbine power plant depends on the fundamental thermodynamics. The thermodynamic cycle simulation shows the limitation of performances due to the first and second laws of thermodynamics. Numerous studies have been conducted regarding the Brayton cycle for improving the thermal efficiency and output power for the industrial gas turbine; however, for micro gas turbine, less than 10 kW has very few research outputs [7-9].

There are numerous advantages in terms of efficiency and cost by the methods of optimizing thermodynamic cycle. In this study, a novel method of studying mass flow rate and fuel is considered as a hot working fluid. The hot working fluid study helps in optimizing thermodynamic cycle variables such as temperature and pressure of the micro gas turbine power plant. The combination of Quantum chemistry analysis to study the hot fuel and the basic thermodynamic equations that studies the working fluid helps in modeling better efficient gas turbine engines. The analysis helps in integration of fuel and working fluid as a hot working fluid thus solving the problem of integrating the Combustion chamber with thermomachinery components.

The mathematical model comprises of the Total pressure, Mass flow rate and Peak Temperature. The turbomachinery components consist of the Compressor, Combustor, Turbine and Free Turbine. A hot flow process through a pipe is considered to determine the relationship between Thermal Efficiency, Compressor Pressure ratio, and Power Output. Numerical predictors for net power output was evaluated by studying the effects of hot fluid mass flow rate and drop in pressure drops as shown in figure 1.

![Figure 1. Optimizing Thermodynamic Cycle Calculation (TCC)](image-url)
flow process through a pipe is considered to determine the relationship between Thermal Efficiency, Compressor Pressure ratio, and Power Output. Numerical predictor for net power output was evaluated by studying the effects of hot fluid mass flow rate and drop in pressure drops.

An optimization model created combines the heat from combustion chamber integrated with the working fluid by considering the system as a hot pipe. The study helps in improving the existing models of designing a gas turbine power plant focused on improving the efficiency of the power output generated.

Various researches for the search in alternative fuels has led to Dimethyl ether as expressed in chemical terms (DME; formula: CH$_3$-O-CH$_3$). The property of DME has resulted to be highly valued [10]. The DME has the interesting property of containing low traces of octane. Various experiments have been published of using DME for combustion to have resulted in low pollutant emission which is one of the main reasons to perform a parametric investigation on micro gas turbine fuelled by DME. The Main research work deals with investigating the kinetics and mechanism of the following reaction (A) in the temperature range 800–1350 K at an optimized total pressure similar to high altitude flights.

$$\text{C}_2\text{H}_6\text{O} + 3^*(\text{O}_2+3.76) \text{N}_2 \rightarrow 2\text{CO}_2 + 3\text{H}_2\text{O} + 11.3\text{N}_2 \quad ----- \quad \text{(A)}$$

$$\text{CH}_3\text{OCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{OCH}_2 + \text{H}_2\text{O} \quad ----- \quad \text{(B)}$$

Whereas, the transition state during the combustion process is denoted by

$$\text{CH}_3\text{OCH}_2\text{O}^\# \quad ----- \quad \text{(C)}$$

The results obtained are used to perform parametric analysis for a 300W micro gas turbine power plant. The complete combustion reaction of DME in the presence of air similar to gas turbine combustion process is represented as equation (A). However, the DME gets oxidized in the troposphere region into methoxymethyl radical in the presence of hydroxyl radicals the reaction shown in equation (B) [11-12].
In modern quantum chemistry applications, geometry optimizations for very large molecules are possible due to advancement in computing power and efficient density functional theory methods (DFT). The density functional theory program demon discusses the geometry optimization for the selection of coordinates in space. The trust radius of the element is selected based on Cartesian geometry change for optimization with the influence of the self-consistent field (SCF) convergence [13]. To design any micro gas turbine power systems, a prerequisite pre-phase design review is necessary. The studies define the operational requirement of the system. The Gas turbine power plant operates in the principle of the Brayton cycle and a representation is shown in figure 3. The micro gas turbine power plant has an Intake, Centrifugal compressor, Combustor, first turbine to run the compressor, free turbine connected to the generator via shaft and exhaust.

![Figure 3. The model of the gas turbine power plant.](image)

The station numbering process helps in understanding the thermodynamic cycle of the engine in the Brayton cycle is clearer. The process on the p-V or T-s diagram should be numbered as described in the station numbering system. To avoid design complexity in the design of Gas turbine, it is necessary to be represented in schematics for simplified understandings. The schematic of our engine is represented in figure 3 [14].

### Table 1. Power plant input parameters

| Parameters                        | Values          |
|-----------------------------------|-----------------|
| Compressor type                   | Centrifugal     |
| The overall pressure ratio of the compressor. | 3               |
| Stagnation temperature at turbine inlet | 1500 K         |
| Turbine Type.                     | Axial           |
| Excess power capacity on the rotor shaft for generator output. | 6kW             |
| Composition and properties of the fuel. | Kerosene, T1   |

### 5. RESULTS AND DISCUSSIONS

This multi-model optimization process of analyzing the performance of thermal efficiency and Power density helps in solving an engineering problem. The model determines joint parametric analysis for improvement in thermal efficiency from both thermodynamic calculations and quantum level accuracy. Multi-objective optimization helps in integrating countless sets of equations and functions. Many cases have been reported to use multi-objective optimization, however, in this research, it has been used to optimize the thermal and overall efficiency of the micro gas turbine power plant. In a similar cycle analysis for repetitive calculation Genetic Algorithm can also be used. [15]. The design
of the micro gas turbine power plant was fixed at 6kW constant power output and the combustion and emission characteristics were varied by the fuel-air mixing process and combustion characteristic. The reactants and products of the DME molecule combustion in the presence of air similar to high altitudes were analyzed using Normal coordinate and Ab initio SCF calculations. The calculated values were simulated and obtained for the least vibrational amplitudes along with the zero-point energy difference energy values. The process of ab initio geometry optimization of the chemical kinetics errors is represented by uncertainties. The supercomputers help us to predict with high accuracy properties of thermodynamic calculation and convergence at less time. The following figure 4 helps to model the fuel along the temperature pattern for optimum combustion methods.

![Figure 4. Temperature influence on the fuel at the molecule level.](image1)

The rate of the combustion reaction of DME changes with the concentration of fuel in the mass flow rate hence the reaction products depend on the pressure ratio of the compressor. The working fluid could be modeled as mixtures of fuel–oxygen and fuel-air mixtures. The high and low altitude influence on fuel combustion helps in designing the combustion chamber peak temperature cycle as the combustion temperature reaches maximum 1300 degree Celsius. The values of activation energy of the reactants and products of equation A is shown in figure 5.

![Figure 5. The activation energy of the reaction.](image2)

Research on DME chemical kinetics of obtaining rate constant resulted in NO change with the pressure of the DME [16], however, in Gas turbine engine the DME is mixed working fluid atmospheric air and this pressure changes the Rate constant of the entire system due to the multi-complex determination of the reactants. Our Theoretical model values are (+/-) 2% equivalent to the experimental values obtained in the reference [17]. The research concluded by examining the numerical model to calculate the thermodynamic parameters of DME for a micro gas turbine power plant based on the assumption of input parameters similar to that of high altitude flight. The results show the differences in the conventional method with the integration of quantum techniques. The rate of the combustion reaction of DME changes with the concentration of fuel in the mass flow rate of the working fluid. The specific fuel consumption increases with a mass flow rate of the working fuel. The fuel mass flow rate increases with the increase in the mass flow rate of the working fuel. The mass flow rate depends on the pressure ratio of the compressor. The chemical reaction obtained products depend on the pressure ratio of the compressor. The working fluid could be modeled as mixtures of fuel–oxygen or fuel-air mixtures. At high altitudes, both of these models need to be studied as the altitude increases oxygen content in the working fuel decreases due to the ambient conditions. For the conventional engine, about 36% improvement in merit value was achieved during the optimization process from the baseline to the optimized design.

Initial condition with respect to the overall model of the gas turbine power plant represented graphically with zoomed up values. The turbine inlet temperature (TiT) expressed in K. The chemical kinetics models of the reaction of DME helps in better analysis and design for geometries of the combustion chamber for the micro gas turbine power plant. The dynamics of chemical kinetics in the reaction has to be calculated for thermodynamic expansion of the gas. The solution solving process of the gas dynamic equation is time-consuming hence requires supercomputer facilities. The design impacted the size, mass and volume of DME powered gas turbine power plant engine was optimized.
The Parametric value obtained after the thermodynamic cycle optimization are depicted as results shown in the figure 6, 7, 8 and 9.

Figure 6. Temperature influence on the fuel at the molecule level.

Figure 7. Pressure ratio influence on efficiency over various temperatures.

Figure 8. Temperature influence on the fuel at the molecule level.

Figure 9. Optimum Mass flow rate for the least specific fuel consumption.

6. References

[1] Zhongyue Xu, Da-Wen Sun, Xin-An Zeng, Dan Liu & Hongbin Pu 2015 Critical Reviews in Food Science and Nutrition. 55:9 1270-1286 DOI: 10.1080/10408398.2013.821593/

[2] Matt Grote, Ian Williams, John Preston, 2014 Atmospheric Environment 95 214-224 ISSN 1352-2310, https://doi.org/10.1016/j.atmosenv.2014.06.042.

[3] Farouk, N., L. Sheng, and Q. Hayat. 2015 International Journal of Computer Science Issues, 10:1.

[4] Kuz'michev V.S., Tkachenko A.Y., Ostapyuk Y.A. etc. 2017 Features of computer modeling of the working process of small-scale gas turbine engines, International Conference on Mechanical, System and Control Engineering, ICMSC 2017. P. 136-140.

[5] Rybakov V.N., Kuz'michev V.S., Tkachenko A.Y. etc. 2016 Thermodynamic multi-criteria optimization of the unified engine core for the line of turbofan engines Proceedings of the ASME Turbo Expo. Vol. 1.

[6] Tkachenko A.Y., Kuz'michev V.S., Krupenich I. N. etc. 2016 Gas Turbine Engine Optimization at Conceptual Designing MATEC Web of Conferences. Vol. 77.

[7] Kuz'michev VS , Tkachenko AY , Krupenich IN etc. 2014 Composing a virtual model of gas turbine engine working process using the CAE system "ASTRA" Research Journal of Applied Sciences Vol. 9. Issue 10. - P. 635-643.

[8] Kuz'michev VS , Rybalko VN , Tkachenko AY etc. 2014 Optimization of the working process
parameters of gas turbine engines *ARPN Journal of Engineering and Applied Sciences* Vol. 9, Issue 10. - P. 1873-1878.

[9] Bang T. Diep, and Mark S. Wainwright, 1987, *J. Chem. Eng. Data*, 32 (3), pp 330–333 DOI: 10.1021/je00049a015

[10] Roman Wrobel, Wolfram Sander, Elfi Kraka and Dieter Cremer 1999 *J. Phys. Chem. A*, 103, 3693-3705.

[11] Peng Zhang, Shuang Li, and et all, 2017, *Combustion and Flame*, 183, Pages 30-38, ISSN 0010- 2180, https://doi.org/10.1016/j.combustflame.2017.05.006.

[12] A. Perry, R. Atkinson, and J. N. Pitts 1977 *The Journal of Chemical Physics* 67, 611 doi: 10.1063/1.434862 View online: https://doi.org/10.1063/1.434862

[13] Reveles JU1, Köster AM. 2004 *J Comput Chem.* 15; 25(9): 1109-16.

[14] Jeffryes W. Chapman, Thomas M. Lavelle and Jonathan S 2016, *NASA/TM 2016-219147*.

[15] Mohammad Hossein Ahmadi Mohammad Ali Ahmadi Arash Shafaei and et all, 2016 *International Journal of Low-Carbon Technologies*, Volume 11, Issue 3, 1 Pages 317–324, https://doi.org/10.1093/ijlct/ctv001

[16] Takahashi K, Yamamoto et all, 2007 *Int. J. Chem. Kinet.* 39 (97 - 108).

[17] Tsang, W, *Inter. J. Chem. Kinet.* 2004. 36 (456 - 465).

[18] Patten J, McWha T. 2015 National Research Council Canada. Automotive and Surface Transportation 10.4224/23000192.

[19] Glaude PA, Fournet R, Bounaceur R, Molière M. DME as a Potential Alternative Fuel for Gas Turbines: A Numerical Approach to Combustion and Oxidation Kinetics. ASME. Turbo Expo: Power for Land, Sea, and Air, *Volume I*: Aircraft Engine; Ceramics; Coal, Biomass and Alternative Fuels; Wind Turbine Technology:649-658. doi:10.1115/GT2011-46238.

[20] MATSUMOTO, Ryosuke & IMAHORI, Keizo & TAKAICHI, Katsuhiko & ISHIHARA, Isao & OZAWA, Mamoru. (2003). The Proceedings of the Thermal Engineering Conference. 5-6. 10.1299/jismeted.2003.5.

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