Effects of Chemical Equilibrium on Turbine Engine Performance for Various Fuels and Combustor Temperatures

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PERFORMANCE FOR VARIOUS FUELS AND COMBUSTOR TEMPERATURES

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SUMMARY

A study was performed to quantify the differences in turbine engine performance with and without the chemical dissociation effects for various fuel types over a range of combustor temperatures. Both turbojet and turbofan engines were studied with hydrocarbon fuels and cryogenic, nonhydrocarbon fuels. Results of the study indicate that accuracy of engine performance decreases when nonhydrocarbon fuels are used, especially at high temperatures where chemical dissociation becomes more significant. For instance, the deviation in net thrust for liquid hydrogen fuel can become as high as 20 percent at 4160 °R. This study reveals that computer central processing unit (CPU) time increases significantly when dissociation effects are included in the cycle analysis.

1.0 INTRODUCTION

The Navy/NASA Engine Program (NNEP) (ref. 1) is a computer program that was developed in 1975 to calculate the thermodynamic cycle performance of different turbine engines ranging from subsonic turboprops to variable-cycle engines for supersonic transports. However, there were certain thermodynamic cycles that NNEP was not capable of modeling efficiently. These deficiencies included the use of cryogenic or nonhydrocarbon fuels and chemical dissociation effects that occurred as engine cycles were operated at high temperatures. Several algorithms were evaluated to improve the thermodynamic modeling in NNEP. The procedure chosen was a computer program for calculation of chemical equilibrium compositions (CEC), which was first written in 1961 (ref. 2). Later, CEC went through numerous changes to increase its capabilities, flexibility, and speed. After these changes, the CEC program was incorporated into NNEP to more accurately calculate the engine performance, including the effect of chemical dissociation and the use of nontraditional fuels. This new program is now called the NASA Engine Performance Program (NEPP). The details and interfacing of the NNEP and CEC programs are discussed in references 3 to 5.

The purpose of this study was to quantify the differences in engine performance with and without the chemical dissociation effects (i.e., with and without CEC). Three engine cycles were evaluated with several fuels over a range of combustor temperatures. Computer central processing unit (CPU) time was also assessed. Major differences in engine performance that were caused by chemical dissociation effects and the changes in computer time will be discussed.

2.0 DISCUSSION AND METHOD OF ANALYSIS

The engine performance was calculated by the NEPP code. Engine parameters assessed included net thrust, combustor fuel-to-air ratio, inlet-corrected weight flow, and thrust specific fuel consumption (TSFC). Each engine was sized for 100-lbm/sec inlet-corrected weight flow at the design point. The engine performance calculated with CEC was chosen to be the baseline, and the deviation was determined
from the performance calculated without CEC. For each engine parameter, the deviation was determined by the following equation:

\[
\text{Percent deviation} = (1.0 - \frac{\text{Answer without CEC}}{\text{Answer with CEC}}) \times 100 \text{ percent}
\]

For thermodynamic data, NEPP uses either the THERM or THERME subroutine. These subroutines are discussed and compared next. Then chemical dissociation is discussed, and the test matrix is presented.

2.1 THERM and THERME Subroutines

THERM, the default NEPP thermodynamic subroutine, contains cubic spline curve fits of thermodynamic data for a default hydrocarbon fuel with a hydrogen-to-carbon ratio of 0.16 and a heating value of 18,500 Btu/lb. THERM assumes that the thermodynamic properties of a gas stream are a function of its temperature only (no pressure effects) and are calculated as a linear combination of air and stoichiometric products. THERM is accurate for estimating gas thermodynamic properties if the fuel is similar to the default fuel and if the engine cycle is operated at conditions that involve little chemical dissociation. To maintain accuracy when using a fuel different from the default, one must incorporate the proper data tables in the THERM subroutine for that specific fuel and air combination. However, chemical dissociation cannot be modeled accurately because pressure effects are not accounted for.

A new subroutine, THERME, was developed to incorporate equilibrium effects into NEPP. THERME calls the CEC program (rewritten as a subroutine to THERME) to get equilibrium properties. The CEC program also uses curve fits of thermodynamic data for all possible chemical species; these curve fits can be input in a standard form as described in reference 2. The CEC program determines which species are present and their relative amounts, assuming equilibrium occurs at the minimum Gibbs free energy point. Once it has determined the equilibrium composition, it then calculates the thermodynamic properties.

Determining the equilibrium composition involves solving nonlinear sets of equations; therefore, more CPU time is required with the THERME subroutine than with the THERM subroutine. However, the changes required to model the fuels other than the default are much simpler with the THERME subroutine and CEC program. These changes can be as minor as changing a line in the input data set. For the THERM subroutine, new thermodynamic data tables have to be calculated and then incorporated into the subroutine.

Both thermodynamic subroutines make simplifying assumptions that may introduce inaccuracies in determining the thermodynamic properties of an engine cycle. They neglect chemical reaction rate effects and assume that the gas stream is always at the equilibrium condition. These assumptions may affect the validity of the solution, depending on the engine type and its operating conditions.

2.2 Chemical Dissociation

Chemical dissociation generally occurs at higher temperatures and lower pressures. During chemical dissociation, the temperature and pressure effects drive the chemical reactions to smaller but higher energy species. Therefore, for a given energy level, chemical dissociation decreases the mixture's temperature and molecular weights, but it increases the specific heat. In an engine cycle, these effects are seen in several components. More fuel must be added in the combustor to reach a desired temperature. This extra fuel may be a small quantity in comparison to the total mass airflow; however, it may change the
mixture’s thermodynamic properties significantly. Inversely, if chemical dissociation is reduced by decreasing temperature or increasing pressure, the species recombine into higher molecular weights and lower energy products. This recombination reduces the turbine pressure ratio for a required amount of work, and it may increase the nozzle exit pressure and jet velocity, thereby increasing the engine’s thrust.

2.3 Test Matrix

The test matrix used for the study is shown in table I. Three types of engines were run with three different fuels at three different combustor temperatures. The engine performance was calculated with and without CEC. It was also calculated in a combination running mode without and then with CEC, in an attempt to reduce CPU time. However, this option resulted in convergence problems for several cases, with little or no improvement in CPU time in comparison to running with CEC only. Consequently, this option was not considered viable for the duration of the study.

A single-spool turbojet engine and two types of two-spool turbofan engines (separate and mixed flow) were selected for the study. Each engine was “flown” over a typical flight path, for a particular fuel, at a specified combustor temperature with and without CEC. The fuels chosen were two hydrocarbon fuels (JP4 and liquid methane) and a cryogenic, nonhydrocarbon fuel (liquid hydrogen). These fuels were used to determine the deviations caused by using fuels different from the default fuel in the THERM subroutine. The heating values were 18 600 Btu/lb for JP4, 22 219 Btu/lb for liquid methane, and 50 664 Btu/lb for liquid hydrogen. These heating values were calculated with the stand-alone version of the CEC program. Engine combustor exit temperatures of 3460, 3860, and 4160 °R were specified for each fuel to determine the dissociation effects.

3.0 RESULTS AND DISCUSSION

The deviation in engine performance parameters for cases with and without CEC are presented and discussed separately for each engine. A positive deviation means that the case without CEC underpredicted the performance parameter of the case with CEC, and a negative deviation means that it overpredicted the value. The differences in engine performance parameters between cases with and without CEC occurred for two reasons.

(1) The THERM subroutine was unable to model the changes in the chemical system properly because the fuel used was not the default fuel. In this study, it was decided to use the default tables and to change the fuel heating value only. This was a worst case scenario, but it would be informative to someone who needed immediate answers and who did not have the time to run the CEC option or to change the THERM data tables.

(2) Inclusion of the chemical dissociation effects altered the calculated engine performance parameters.

The goal of the study was to show where the fuel and chemical dissociation effects could be neglected and where they could cause significant differences in the engine performance calculations. In the latter case, the CEC option should be activated to prevent large differences. For each engine performance parameter, a maximum deviation was determined for the off-design conditions for a particular fuel and combustor temperature combination. These maximum deviations then were plotted versus fuel types and combustor temperatures. The study showed that whereas some engine parameter deviations depended on the engine cycle, others did not. Therefore, these results should be used only as a
guideline as when to run with CEC. Users should be very cautious not to apply “fudge factors,” using these results to correct for the chemical dissociation and fuel effects relative to their particular applications. The effects of running with CEC in terms of CPU time are discussed last.

3.1 Single-Spool Turbojet Engine

The flight path used for the single-spool turbojet is shown in table II, and a schematic for this engine with the design point parameters is presented in figure 1. The design point was sea level static. A converging-diverging nozzle was assumed. The nozzle throat area was kept constant, and full nozzle expansion was assumed. Typical component maps were used to model the compressor and turbine off-design performance.

3.1.1 Net thrust.—For the turbojet engine, with any fuel, increasing the design point combustor temperature increased the net thrust. Also, reducing the carbon-to-hydrogen ratio of the fuel reduced the molecular weights of the combustion products, further increasing the net thrust. Figure 2 shows a plot of net thrust versus Mach number calculated by CEC for three different fuels at a combustor temperature of 4160 °R. The net thrusts were highest for liquid hydrogen, followed by liquid methane and JP4 fuels. This hierarchy occurred because of the lower molecular weights of the combustion products and the higher specific heat, causing a smaller pressure drop across the turbine and a resulting higher nozzle exit jet velocity.

The more the fuel deviated from the THERM default fuel, or the more the combustor temperatures increased, the greater the deviation in net thrust. Figure 3 shows the maximum deviation in net thrust versus combustor temperature for all fuels. Liquid hydrogen had the largest deviations over the range of combustor temperatures. The maximum deviation in net thrust for liquid hydrogen ranged between 13.6 to 17.8 percent, with the largest deviation occurring at the highest combustor temperature. The deviation for liquid methane was not as large as for the liquid hydrogen, but it still ranged from 5.3 to 7.7 percent. For JP4, the THERM subroutine showed good agreement with the CEC results with the difference ranging only from 1.5 to 2.8 percent.

3.1.2 Combustor fuel-to-air ratio.—For all the fuels, engine fuel flow increased with increasing combustor temperature. Figure 4 presents the combustor fuel-to-air ratio deviations for all fuels. There were some differences with JP4; however, the largest differences in the fuel-to-air ratio occurred when liquid hydrogen was used. This happened because the THERM subroutine was written for hydrocarbon fuels, and it underpredicted the increase in the specific heat of the combustion products, especially at higher combustor temperatures. The effects of chemical dissociation could be seen as the deviation increased with increasing temperature along the curve for each fuel. The effect of various fuels (effect of difference from the default hydrogen-to-carbon fuel ratio) was illustrated by the magnitudes of the differences that made up the curves.

The maximum deviation in fuel-to-air ratio for liquid hydrogen ranged from 15.3 to 21.9 percent, with the largest difference occurring at the highest combustor temperature. The maximum deviation in fuel-to-air ratio for liquid methane ranged from 6.0 to 10.0 percent. The deviation in fuel-to-air ratio was smallest for JP4, with the maximum difference ranging from 1.4 to 4.1 percent. The shapes of the combustor fuel-to-air ratio deviation curves indicate that, when running the program without CEC, the fuel heating value should be input as a function of combustor entrance and/or exit temperatures instead of as a constant.
3.1.3 Inlet-corrected weight flow.—Figure 5 is a typical plot of the inlet-corrected weight flow for the single-spool turbojet engine using liquid hydrogen at all combustor temperatures with and without CEC. As can be seen, all six curves fell nearly upon one line. The inlet-corrected weight flow was hardly affected by combustor temperature or chemical dissociation. (Differences are less than 0.1 percent.) The differences for liquid methane and JP4 were similar, so these graphs were not included.

3.1.4 Thrust specific fuel consumption.—Figure 6 shows the maximum deviation in TSFC versus combustor temperature for all the fuels. The maximum deviation in TSFC for liquid hydrogen ranged from 6.9 to 10.9 percent, with the largest difference occurring at the highest combustor temperature. The maximum deviation in TSFC for liquid methane ranged from 2.4 to 4.7 percent. For JP4, the THERM subroutine showed good agreement with CEC results, with the maximum deviation ranging from 0.4 to 1.7 percent.

For all combustor temperatures, the TSFC for JP4 was higher than for the other fuels because of its lower heating value. However, the deviation in the combustor fuel-to-air ratio offset the difference in net thrust, thereby reducing the deviation in TSFC. Still, there were sizeable deviations for the liquid methane and hydrogen fuels.

3.2 Two-Spool, Separate-Flow Turbofan Engine

The flight path for the two-spool, separate-flow turbofan engine is listed in table III, and a schematic for the engine with the design point parameters is shown in figure 7. The design point was sea level static. The design point bypass ratios of this engine, for the purpose of convenience, were the same as those of the two-spool, mixed-flow turbofan engine (which is discussed next) with CEC for all combinations of fuels and combustor temperatures. The design point bypass ratio was the same for cases with and without CEC for a particular combination of fuel and combustor temperature. However, this bypass ratio varied for different combinations of fuels and combustor temperatures from 1.6 for JP4 at 3460 °R to 3.6 for liquid hydrogen at 4160 °R. Converging-diverging nozzles were assumed. Nozzle throat areas were kept constant, and full nozzle expansion was assumed. Typical component maps were used to model the fan, compressor, and turbine off-design performance.

3.2.1 Net thrust.—It was found earlier (section 3.1.1) that for a turbojet engine, the net thrust with CEC was highest for liquid hydrogen followed by liquid methane and JP4 fuels for the same inlet-corrected weight flow. For the two-spool, separate-flow turbofan engine, the bypass ratio was highest for liquid hydrogen, because of a higher specific heat, followed by liquid methane and JP4 fuels. Figure 8 shows that the net thrust with CEC for JP4 was slightly higher than for liquid methane and liquid hydrogen fuels at 4160 °R. In spite of the higher bypass ratio of the hydrogen-fueled turbofan, the net thrust is practically equal to that of the JP4-fueled turbofan. This is attributed to the higher energy available in the hydrogen fuel and air mixture. This tendency also is true for other combustor temperatures.

Figure 9 shows the maximum deviation in net thrust versus combustor temperature for all fuels. The maximum deviation in net thrust ranged from 15.2 to 19.8 percent for liquid hydrogen and from 5.8 to 8.6 percent for liquid methane. For JP4, the THERM subroutine showed good agreement with the CEC option over the entire temperature range. The maximum deviation ranged from 1.3 to 3.0 percent only.

3.2.2 Combustor fuel-to-air ratio.—The calculated combustor fuel-to-air ratios for this engine were very similar to those for the single-spool turbojet engine. This was not totally unexpected, but it was
thought that fuel and dissociation effects might change the engine off-design operating points sufficiently to alter the combustor fuel-to-air ratio. An interesting side note is that, unlike the single-spool turbojet engine, the overall engine fuel-to-air ratio decreased with increasing combustor temperature. This was due to the design point bypass ratio increasing with increasing combustor temperature. The reduction in core airflow was greater than the increase in combustor fuel-to-air ratio.

Figure 10 shows the deviation in the combustor fuel-to-air ratio for all the fuels. Of the three fuels, liquid hydrogen had the largest deviations in the fuel-to-air ratio. The maximum deviation in fuel-to-air ratio for liquid hydrogen ranged from 15.6 to 21.9 percent, with the largest difference occurring at the highest combustor temperature. The maximum deviation in fuel-to-air ratio for liquid methane ranged from 6.1 to 9.8 percent. The deviation in combustor fuel-to-air ratio for JP4 was the smallest, with the maximum deviation ranging from 1.4 to 3.6 percent. The shapes of the combustor fuel-to-air ratio curves were very similar to the trends noted in section 3.1.2.

3.2.3 Inlet-corrected weight flow. — Figure 11 is a plot of the inlet-corrected weight flow for all combustor temperatures for the two-spool, separate-flow turbofan engine using liquid hydrogen with and without CEC. Even though the design point bypass ratio varied with combustor temperature, little or no change was seen in the inlet-corrected weight flow below Mach 1.5. The difference increased above Mach 1.5, but even at the highest point it was minor (less than 1 percent). This trend was similar for liquid-methane-fueled and JP4-fueled engines; therefore, these plots were not included.

3.2.4 Thrust specific fuel combustion. — Since TSFC is directly related to net thrust and the deviations in net thrust were significant for liquid methane and liquid hydrogen fuels, one would expect that the deviations in TSFC would be significant for these fuels too. The deviations in TSFC for all the fuels are shown in figure 12. Liquid hydrogen had the greatest differences in TSFC in comparison to the other fuels. The maximum deviation in TSFC ranged from 6.0 to 10.8 percent for liquid hydrogen, from 2.3 to 4.8 percent for liquid methane, and from 0.5 to 1.7 percent for JP4. Overall, the variations of engine parameters for the two-spool, separate flow turbofan engine were very similar to those for the single-spool turbojet engine.

3.3 Two-Spool, Mixed-Flow Turbofan Engine

The flight path for the two-spool, mixed-flow turbofan engine was the same as for the two-spool, separate-flow turbofan engine (table III). A schematic for this engine with the design point parameters is shown in figure 13. The design point was sea level static. The design point engine bypass ratios for each combination of fuel and combustor temperature running with and without CEC were determined by including the design point cycle constraint of having equal Mach numbers at the mixer entrance (nearly equal total pressures). To meet this requirement, the design point bypass ratio was different for cases with and without CEC. Again, the design point engine bypass ratios varied from 1.4 to 3.6 for different combinations of fuels and combustor temperatures. Engine bypass ratio increased with increasing combustor temperature and was higher for cases with CEC than for cases without CEC for the same combination of fuel and combustor temperature. A converging-diverging nozzle was assumed. The nozzle throat area was kept constant, and full nozzle expansion was assumed. Typical component maps were used to model the fan, compressor, and turbine off-design performance.

3.3.1 Net thrust. — For this engine, with and without CEC, increasing combustor temperature increased the bypass ratio. Less air went through the combustor and less fuel was burned. Still, static pressures at the mixer entrance had to be maintained equal to ensure proper mixing.
As shown in figure 14, the net thrust with CEC using JP4 fuel is slightly higher than with the other fuels at 4160 °R. The reason for this is similar to that for the two-spool, separate-flow turbofan engine, as discussed in section 3.2.1. Figure 15 shows the deviation in net thrust versus combustor temperature for all fuels. The maximum deviation in net thrust for liquid hydrogen ranged from -7.2 to -8.6 percent. The negative sign indicates that net thrust calculated with CEC was less than that without CEC. Meanwhile, the maximum deviation in net thrust ranged from -1.7 to -2.4 percent for liquid methane and from 0.2 to 1.2 percent for JP4. For JP4, net thrust for cases with and without CEC did not differ significantly.

When all engine cycle parameters remained the same, running with CEC increased the net thrust, as seen for the turbojet and separate-flow turbofan engines. For the mixed-flow turbofan when running with CEC, the energy of the core stream increased resulting in a higher bypass ratio than running without CEC. Increasing the bypass ratio at constant engine airflow and fan and compressor pressure ratios reduced the net thrust. The net result of the increase in net thrust from running with CEC and of the reduction in net thrust from the increase in engine bypass ratio was that the deviation in net thrust can be either a positive or negative value, as seen here.

The deviation in net thrust was smaller for the mixed-flow turbofan than for the turbojet and separate-flow turbofan engines. This was due to the compensating effect of chemical dissociation and the bypass ratio, which tended to limit the increase in net thrust when running with CEC. Therefore, there was less difference in net thrust for the two-spool, mixed-flow turbofan. If the design point bypass ratios with and without CEC were the same for the two-spool, mixed-flow turbofan engine, the deviations in engine performance parameters would increase even more, and the trends would be similar to those for the two-spool, separate-flow turbofan engine.

3.3.2 Combustor fuel-to-air ratio.—Figure 16 shows the deviation in the combustor fuel-to-air ratio for all the fuels. The trends were similar to the previous plots for the single-spool turbojet and two-spool, separate-flow turbofan engines, as discussed in sections 3.1.2 and 3.2.2. Liquid hydrogen had the largest deviations in the combustor fuel-to-air ratio. The maximum deviation ranged from 16.0 to 22.6 percent, with the largest difference occurring at the highest combustor temperature. The maximum deviation ranged from 6.2 to 10.2 percent for liquid methane and from 1.3 to 3.8 percent for JP4.

3.3.3 Inlet-corrected weight flow.—There was a small change in the inlet-corrected weight flow (less than 1 percent) with and without CEC at Mach 1.8 and above for all the fuels at all combustor temperatures. The trend for the liquid-hydrogen-fueled engine can be seen in figure 17. The plots for liquid methane and JP4 were very similar; therefore, they were not included.

3.3.4 Thrust specific fuel consumption.—The maximum deviations in TSFC for all the fuels over a range of combustor temperatures are shown in figure 18. It was noted that the deviations in TSFC decreased at higher combustor temperatures for liquid methane and liquid hydrogen because of the fuel flow and net thrust values. The maximum deviation in TSFC ranged from -2.2 to -3.9 percent for liquid hydrogen and from -0.5 to -1.2 percent for liquid methane. For JP4, the maximum deviation was insignificant (less than 0.3 percent).

For all the fuels at all combustor temperatures, the bypass ratio and combustor fuel-to-air ratio with CEC were higher than without CEC. For JP4, the engine fuel flow with CEC was almost identical to the engine fuel flow without CEC. The maximum deviation in TSFC (engine fuel flow divided by net thrust) was small because there was not much difference in fuel flow and net thrust.
3.4 Two-Spool, Mixed-Flow Turbofan Engine With Mixer Optimization

The flight path for the two-spool, mixed-flow turbofan engine with mixer optimization was the same as for the two-spool, separate-flow turbofan engine (table III). The engine was configured the same as for the previously discussed two-spool, mixed-flow turbofan engine (see section 3.3). The only difference between this engine and the previous one was that the optimization feature in NEPP was employed to vary the mixer secondary inlet geometry to minimize TSFC. The total area of the mixer (primary plus secondary areas), however, was constant for all off-design cases.

3.4.1 Net thrust.—Again, as shown in figure 19, the net thrust for JP4 fuel was slightly higher than for other fuels at 4160 °R for a reason very similar to that discussed in sections 3.2.1 and 3.3.1. This was true for all combustor temperatures.

Figure 20 shows the deviations in net thrust versus combustor temperature for all the fuels. The maximum deviation in net thrust ranged from -1.75 to -6.2 percent for liquid hydrogen, from -1.11 to 1.11 percent for liquid methane, and from 0.4 to 1.5 percent for JP4. The reasons for the differences in net thrust were the same as those for the two-spool, mixed-flow turbofan engine without optimization, as discussed in section 3.3.1.

3.4.2 Combustor fuel-to-air ratio.—Figure 21 shows the deviations of the combustor fuel-to-air ratio. This figure has the same trends as figures 4, 10, and 16, as discussed in sections 3.1.2, 3.2.2, and 3.3.2, respectively. Liquid hydrogen had the largest deviations in the combustor fuel-to-air ratio. The maximum deviation ranged from 15.8 to 21.8 percent, with the largest deviation occurring at the highest combustor temperature. The maximum deviation ranged from 5.9 to 9.8 percent for liquid methane and from 1.3 to 3.7 percent for JP4.

3.4.3 Inlet-corrected weight flow.—For all fuels at all combustor temperatures, there was only a small difference in the inlet-corrected weight flow (less than 1 percent) between cases with and without CEC at Mach 1.8 and above. This trend for the liquid-hydrogen-fueled engine can be seen in figure 22. The plots for liquid methane and JP4 were very similar; therefore, they were not included.

3.4.4 Thrust specific fuel consumption.—The deviations in TSFC for all the fuels over a range of combustor temperatures are shown in figure 23. The maximum deviation in TSFC ranged from -2.2 to -3.9 percent for liquid hydrogen, from -0.54 to -1.28 percent for liquid methane, and from 0.01 to 0.25 percent for JP4. These results are very similar to those for the two-spool, mixed-flow turbofan engine without optimization (section 3.3.4).

3.5 Computer Time (CPU)

From this study, running the engine cycles with CEC took more CPU time than without CEC because the program had to perform more calculations to obtain the thermodynamic properties. The difference in CPU time between cases with and without CEC depended on the complexity of the chemical system and engine cycle. The study was performed with an Amdahl 5860 computer running with the Virtual Machine/System Product (VM/SP release 4) Operating System.

Figure 24 shows the range of ratios of CPU time running with and without CEC versus fuel types for the turbojet engine at 4160 °R. As the chemical system increased in complexity, so did the ratio of CPU time. Liquid hydrogen had the simplest chemical system; therefore, it had the lowest ratio of CPU times. Liquid methane and JP4, on the other hand, had fairly similar ratios of CPU times. This was
expected because both fuels contained only hydrogen and carbon atoms. The CPU time increased slightly for JP4 in comparison to liquid methane because the JP4-fueled engine was running at close to stoichiometric conditions at higher combustor temperatures. These conditions tended to increase the number of intermediate species that had to be accounted for in the chemical equilibrium calculations.

Figure 25 shows the effect of engine types in terms of the ratio of CPU times for cases with and without CEC for all the fuels and combustor temperatures. It indicates that as the engine cycle calculations became more complex, the ratio of CPU time increased. The two-spool, mixed-flow turbofan engine with mixer optimization had the highest maximum and minimum ratios of CPU time because of the amount of time spent in the CEC program.

4.0 SUMMARY AND CONCLUSIONS

The NASA Engine Performance Program (NEPP) was applied in this study to determine the differences in turbine engine performance and computer time with and without the use of the chemical equilibrium (CEC) option. The modeled engines were a one-spool turbojet, a two-spool, separate-flow turbofan, and a two-spool, mixed-flow turbofan. The fuels chosen were a “standard” hydrocarbon fuel (JP4) and two nontraditional fuels (liquid methane and liquid hydrogen). Combustor temperatures of 3460, 3860, and 4160 °R were selected to determine the chemical dissociation effects induced by temperature.

The key engine performance parameters evaluated were net thrust, combustor fuel-to-air ratio, inlet-corrected weight flow and net thrust specific fuel consumption (TSFC). The results from the CEC calculations were used as the baseline to determine the percentage deviations from running without CEC. The engine parameters were also calculated by running the engine cycles without CEC and then with CEC during the NEPP iteration process, but this was not a viable option because there were convergence problems and little improvement in CPU time in comparison to running with CEC. Therefore, this option was not considered further. The CPU time required to run the engine with and without CEC was also examined to determine how various engine cycles and fuel types affect the computational process.

For all the engines, the deviations in engine performance parameters were largest for liquid hydrogen followed by liquid methane and JP4 fuels. This hierarchy occurred because as the fuel deviated further from the default fuel in subroutine THERM, the differences in thermodynamics properties increased. Increasing combustor temperature generally increased the deviation in engine performance as a result of chemical dissociation. Either new thermodynamic data tables must be input in the THERM subroutine for other fuel-air combinations, or the CEC option must be activated to obtain more accurate results.

According to these results, the inlet-corrected weight flow over the flight path was almost the same between cases with and without CEC for a particular fuel at all combustor temperatures. This indicates that the inlet-corrected weight flow was not dependent on fuel type and combustor temperature. The deviations in combustor fuel-to-air ratio for all the fuels at various combustor temperatures did not vary greatly from engine to engine. They ranged from 15 to 23 percent for liquid hydrogen, from 6 to 11 percent for liquid methane, and from 1.3 to about 4 percent for JP4. From the shape of the combustor fuel-to-air ratio curve, the users should input the fuel heating value as a function of combustor temperature, rather than as a fixed value for each fuel when running without CEC.

The trends of the results in net thrust and TSFC were very similar for the turbojet and the two-spool, separate-flow turbofan engines. The maximum deviation in net thrust was 20 percent for
liquid hydrogen, 9 percent for liquid methane, and 3 percent for JP4. The maximum deviation in TFSC was 10.9 percent for liquid hydrogen, 4.8 percent for liquid methane, and 1.7 percent for JP4.

For the two-spool, mixed-flow turbofan engines (with and without the optimization feature), the maximum deviation in net thrust was -8.6 percent for liquid hydrogen, -2.4 percent for liquid methane, and 1.5 percent for JP4. The maximum deviation in TSFC was -3.9 percent for liquid hydrogen, -1.2 percent for liquid methane, and 0.25 percent for JP4. The deviations in net thrust and TSFC were smaller for the mixed-flow turbofan engines (with and without optimization control) than they were for the turbojet and separate-flow turbofan engines. When all engine cycle parameters remained the same, running with CEC increased the net thrust. However, for the mixed-flow turbofan, the energy of the core stream increased when running the engine cycles with CEC, resulting in a higher bypass ratio than when running without CEC. Increasing the bypass ratio at constant engine airflow and fan and compressor pressure ratios reduced the net thrust. The net result of the increase in net thrust from running with CEC and the reduction in net thrust from the increase in engine bypass ratio was that the deviation in net thrust was small. Therefore, there were fewer differences in net thrust and TSFC for the two-spool, mixed-flow turbofans. If the design point bypass ratios with and without CEC for the two-spool, mixed-flow turbofan engine were the same, then the deviations in engine performance parameters would increase even more, and the trends would be similar to those for the two-spool, separate-flow turbofan engine.

More CPU time was required to run the engine cycle with CEC than was required without CEC because the CEC program had to solve a set of nonlinear equations to determine the equilibrium composition and then calculate the thermodynamic properties. The ratio of computer time with to without CEC generally was larger for the more complex chemical system (e.g., the JP4 fuel system as opposed to the liquid hydrogen fuel system) because the CEC program had more nonlinear equations to solve. The CPU time also increased with the complexity of the engine cycle. For instance, the ratio of CPU time ranged from 3 for the turbojet to almost 10 for two-spool, mixed-flow turbofan with optimization. This increase in computer time could greatly affect the use of chemical dissociation, and the accuracy of results, for users with limited computer resources.

When running NEPP with liquid methane and liquid hydrogen, the CEC option must be activated to obtain more accurate results on engine performance. Even though this study indicates that for certain engine cycles the deviations with JP4 are fairly small, it does not imply that the users can use the default THERM subroutine on all engine cycles running with JP4. Different engine cycles run with different constraints may give different results. In addition, users should be very cautious not to apply “fudge factors,” using these results to correct for the chemical dissociation and fuel effects relative to their particular applications. The study showed that whereas some engine parameter deviations depended on engine cycle, others did not. Consequently, these results should be used only as a guideline as when to run with CEC. We recommend that users run a representative set of engine test cases with and without CEC to determine whether the CEC option must be used to reach a desired level of accuracy for engine performance.

5.0 REFERENCES


### TABLE I.—ENGINE TEST MATRIX

<table>
<thead>
<tr>
<th>Engine</th>
<th>Chemical equilibrium</th>
<th>Fuel</th>
<th>Combustor temperature, °R</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-spool turbojet</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Two-spool, separate-flow turbofan</td>
<td>Always on</td>
<td>JP4, typical jet fuel</td>
<td>3460</td>
</tr>
<tr>
<td>Two-spool, mixed-flow turbofan</td>
<td>Always off</td>
<td>[H(\text{C}) = 0.16, by mass]</td>
<td>3860</td>
</tr>
<tr>
<td>Two-spool, mixed-flow turbofan with optimization</td>
<td></td>
<td>Liquid methane (CH₄)</td>
<td>4160</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Liquid hydrogen (H₂)</td>
<td></td>
</tr>
</tbody>
</table>

### TABLE II.—FLIGHT PATH FOR SINGLE-SPOOL TURBOJET ENGINE

<table>
<thead>
<tr>
<th>Mach number</th>
<th>Altitude, ft</th>
<th>Mach number</th>
<th>Altitude, ft</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1.5</td>
<td>39 500</td>
</tr>
<tr>
<td>0.26</td>
<td>50</td>
<td>1.8</td>
<td>46 800</td>
</tr>
<tr>
<td>0.60</td>
<td>10 000</td>
<td>2.0</td>
<td>50 900</td>
</tr>
<tr>
<td>0.90</td>
<td>25 000</td>
<td>2.5</td>
<td>55 000</td>
</tr>
<tr>
<td>1.2</td>
<td>32 200</td>
<td>3.0</td>
<td>58 400</td>
</tr>
</tbody>
</table>

### TABLE III.—FLIGHT PATH FOR TWO-SPOOL, SEPARATE-FLOW AND TWO-SPOOL, MIXED-FLOW TURBOFAN ENGINES

<table>
<thead>
<tr>
<th>Mach number</th>
<th>Altitude, ft</th>
<th>Mach number</th>
<th>Altitude, ft</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1.5</td>
<td>39 500</td>
</tr>
<tr>
<td>0.26</td>
<td>50</td>
<td>1.8</td>
<td>46 800</td>
</tr>
<tr>
<td>0.60</td>
<td>10 000</td>
<td>2.0</td>
<td>50 900</td>
</tr>
<tr>
<td>0.90</td>
<td>25 000</td>
<td>2.25</td>
<td>51 500</td>
</tr>
<tr>
<td>1.2</td>
<td>32 200</td>
<td>2.50</td>
<td>52 000</td>
</tr>
</tbody>
</table>
Inlet Corrected weight flow = 100 lb/sec

Compressor
Overall pressure ratio = 12
Efficiency = 85%

Burner
Efficiency = 98%

Turbine
Efficiency = 91%

Cooling bleed

Shaft

Duct

Nozzle

Figure 1.—Single-spool turbojet engine.

Figure 2.—Net thrust for single-spool turbojet engine with CEC (program for calculating chemical equilibrium compositions) at 4160 °R.

Figure 3.—Deviation in net thrust versus combustor temperature for single-spool turbojet engine.
Figure 4.—Deviation in fuel-to-air ratio versus combustor temperature for single-spool turbojet engine.

Computer code | Combustor temperature, °R
--- | ---
△ w/CEC | 3460
O w/o CEC | 3460
◊ w/CEC | 3860
+ w/o CEC | 3860
▼ w/CEC | 4160
□ w/o CEC | 4160

Figure 5.—Inlet-corrected weight flow for single-spool turbojet engine with liquid H₂ fuel.

Figure 6.—Deviation in thrust specific fuel consumption (TSFC) versus combustor temperature for single-spool turbojet engine.
Airflow

Inlet
Corrected weight flow = 100 lb/sec

Fan
Pressure ratio = 3
Efficiency = 84%

Splitter

Compressor
Pressure ratio = 8
Efficiency = 84%

Burner
Efficiency = 98%

Turbine
Efficiency = 91%

Duct

Turbine
Efficiency = 91%

Nozzle

Figure 7.—Two-spool, separate-flow turbofan engine.

Fuel Design point bypass ratio

\[ \begin{align*}
\triangle \text{ JP4} & \quad 2.9856 \\
\bigcirc \text{ Liquid CH}_4 & \quad 3.1924 \\
\square \text{ Liquid H}_2 & \quad 3.6237
\end{align*} \]

Figure 8.—Net thrust for two-spool, separate-flow turbofan engine with CEC at 4160 °R.

Figure 9.—Deviation in net thrust versus combustor temperature for two-spool, separate-flow turbofan engine.
Figure 10.—Deviation in fuel-to-air ratio versus combustor temperature for two-spool, separate-flow turbofan engine.

Figure 11.—Inlet-corrected weight flow for two-spool, separate-flow turbofan engine with liquid H₂ fuel.

Figure 12.—Deviation in TSFC versus combustor temperature for two-spool, separate-flow turbofan engine.
Pressure ratio = 3
Efficiency = 84%

Compressor
Pressure ratio = 8
Efficiency = 84%

Burner
Efficiency = 98%

Turbine
Efficiency = 91%

Mixer
Mach number = 0.3

Nozzle

Figure 13.—Two-spool, mixed-flow turbofan engine.

Figure 14.—Net thrust for two-spool, mixed-flow turbofan engine with CEC at 4160 °R.

Figure 15.—Deviation in net thrust versus combustor temperature for two-spool, mixed-flow turbofan engine.
Figure 16.—Deviation in fuel-to-air ratio versus combustor temperature for two-spool, mixed-flow turbofan engine.

Figure 17.—Inlet-corrected weight flow for two-spool, mixed-flow turbofan engine with liquid H₂ fuel.

Figure 18.—Deviation in TSFC versus combustor temperature for two-spool, mixed-flow turbofan engine.

Figure 19.—Net thrust for two-spool, mixed-flow turbofan engine with mixer optimization with CEC at 4160 °R.
Figure 20.—Deviation in net thrust versus combustor temperature for two-spool, mixed-flow turbofan engine with mixer optimization.

Figure 21.—Deviation in fuel-to-air ratio versus combustor temperature for two-spool, mixed-flow turbofan engine with mixer optimization.

Figure 22.—Inlet-corrected weight flow for two-spool, mixed-flow turbofan engine with mixer optimization with liquid H₂ fuel.

Figure 23.—Deviation in TSFC versus combustor temperature for two-spool, mixed-flow turbofan engine with mixer optimization.
Figure 24.—Effect of fuel type on CPU time for single-spool turbojet engine.

Figure 25.—Effect of engine type on CPU time.
A study was performed to quantify the differences in turbine engine performance with and without the chemical dissociation effects for various fuel types over a range of combustor temperatures. Both turbojet and turbofan engines were studied with hydrocarbon fuels and cryogenic, nonhydrocarbon fuels. Results of the study indicate that accuracy of engine performance decreases when nonhydrocarbon fuels are used, especially at high temperatures where chemical dissociation becomes more significant. For instance, the deviation in net thrust for liquid hydrogen fuel can become as high as 20 percent at 4160 °R. This study reveals that computer central processing unit (CPU) time increases significantly when dissociation effects are included in the cycle analysis.