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INTRODUCTION

Thermodynamic properties for Jet-A fuel are needed for many calculations, including chemical equilibrium calculations. To fulfill this need, various correlations for the estimation of these properties have been published (1,2,3). However, these are difficult to use and may not be practical for all applications. In 1970, Shell Development Company, under a contract for NASA Lewis Research Center, determined the thermodynamic properties for a Jet-A fuel (4). In the present report, we used these thermodynamic data to derive the coefficients necessary to include Jet-A (gaseous and liquid phases) in the thermodynamic data library of the NASA Lewis Chemical Equilibrium Program (5). To verify the thermodynamic data and the polynomial fit, the temperatures of very rich mixtures of Jet-A and nitrogen were measured and compared to those calculated by the chemical equilibrium program.

THERMODYNAMIC DATA AND LEAST SQUARES FIT

To include Jet-A in the thermodynamic data library of the NASA Lewis Chemical Equilibrium Program (5), the thermodynamic functions specific heat C_p° , enthalpy H_T° , and entropy S_T° , need to be expressed as functions of temperature in the form of a fourth order polynomial for C_p° , with integration constants for H_T° and S_T° .

$$\frac{C_p^\circ}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad 1)$$

$$\frac{H_T^\circ}{RT} = a_1 + \frac{a_2 T}{2} + \frac{a_3 T^2}{3} + \frac{a_4 T^3}{4} + \frac{a_5 T^4}{5} + \frac{a_6}{T} \quad 2)$$

$$\frac{S_T^\circ}{R} = a_1 \ln T + a_2 T + \frac{a_3 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7 \quad 3)$$

The thermodynamic data for a Jet-A fuel used for this report were measured or calculated by Shell Development Company in 1970. Most of these data were in an extensive unpublished table provided to NASA Lewis Research Center by Shell. Part of the data contained in this table and additional fuel information used for this report were published in reference 4. The data used from reference 4 include: heat of combustion value used to calculate the heat of formation of the liquid, and a fuel analysis by hydrocarbon type and carbon number used to estimate the entropy of the gaseous fuel mixture at 298K. The data used from the unpublished table include: heat capacity and enthalpy values for gaseous Jet-A for temperatures from 273K to 1273K, the entropy and enthalpy of vaporization at 298K, and enthalpies for liquid Jet-A for temperatures from 220K to 550K. The values for enthalpy given in this table were referenced to liquid Jet-A at 273K. The chemical equilibrium program requires an assigned enthalpy value at 298K equal to the heat of formation. For this reason, the enthalpy values from the unpublished table were adjusted to be relative to the enthalpy at 298K.

The entropy values given in Shell's unpublished table were referenced to liquid Jet-A at 273K. The chemical equilibrium program requires the entropy to be zero at 0 K. To estimate the entropy for the gaseous Jet-A, the fuel analysis given in Table XVI of reference 4 was used along with the entropy values of the individual components from reference 6. The entropy of vaporization at 298K was obtained from Shell's unpublished table and subtracted from the gas phase entropy to obtain the entropy at 298K for the liquid phase.

An updated version of the PAC computer code (7), namely PAC87 was used to extrapolate the thermodynamic functions for the gas to 5000K (8) and fit C_p° and H_T° simultaneously using a least squares method. The data were fitted in two temperature intervals, 298K to 1000K and 1000K to 5000K.

For the liquid Jet-A, the heat capacity values in the unpublished table did not match the enthalpies for temperatures above 600K. Since the enthalpy was the property measured by Shell Development Company (4), it was used in the PAC87 computer code to obtain heat capacity and entropy values for the temperature range 220K to 550K.

The chemical formula $C_{12}H_{23}$ was used to represent Jet-A in the computer program. This results in a molecular weight of 167.3. A value of 166 was reported in reference 4.

The coefficients obtained for the liquid and gaseous phases are the following:

LIQUID: 220K≤T≤550K	GAS: 273K≤T≤1000K	GAS: 1000K≤T≤5000K
a ₁ = 0.19049613E 02	a ₁ = 0.20869217E 01	a ₁ = 0.24880201E 02
a ₂ = -0.16918532E-01	a ₂ = 0.13314965E 00	a ₂ = 0.78250048E-01
a ₃ = 0.63022035E-03	a ₃ = -0.81157452E-04	a ₃ = -0.31550973E-04
a ₄ = -0.13336577E-05	a ₄ = 0.29409286E-07	a ₄ = 0.57878900E-08
a ₅ = 0.94335638E-09	a ₅ = -0.65195213E-11	a ₅ = -0.39827968E-12
a ₆ = -0.44803964E 05	a ₆ = -0.35912814E 05	a ₆ = -0.43110684E 05
a ₇ = -0.67690200E 02	a ₇ = 0.27355289E 02	a ₇ = -0.93655255E 02

VERIFICATION

Experimental Apparatus

Experiments were conducted in the vaporization section of a catalytic flow-tube reactor described in reference 9. Open-end J-type thermocouples were used to monitor the gas mixture temperature. They were located at 46, 53, 61 and 68 cm from the point of fuel injection.

Two fuel injector designs were used in this work (see Figure 1). Both consisted of seven 10-cm long conical nozzles arranged with six in a circle and one in the center. Fuel was delivered to each cone through tubes of equal length and of 0.04 cm ID. These tubes were located to spray the fuel in the direction of the gas flow. The fuel distribution through the fuel injectors was examined and was found to be uniform within 7% for fuel injector A and 4% for fuel injector B. A nitrogen purge in the fuel line was required to remove any residual fuel in the fuel tubes before shut-down. This eliminated clogging of these small tubes.

Operating Procedure

Nitrogen is heated to about 800K with an electric heater. The standard operating procedure was to warm-up the reactor for about two hours with hot nitrogen to attain a steady state temperature. Then, liquid fuel is added and the mixture temperature 68 cm downstream of the point of fuel injection was monitored. No data was recorded until the temperature was steady for about 5 minutes. This took about 30 minutes for the first point. Then the fuel flow was increased or decreased, and data were taken in the same manner. For the second point on, data could be taken every 10 minutes.

Experimental Approach

The objective of this study is to verify the thermodynamic properties of a Jet-A fuel by measuring the temperatures of very rich vaporized fuel/nitrogen mixtures. In a prior study (2) it was observed that the addition of large quantities of liquid fuel to a high temperature gas stream caused a large reduction in the stream temperature (200 to 300K). This mixture temperature can be calculated using the chemical equilibrium program and the thermodynamic properties of the fuel (liquid and gas) and nitrogen. We found that in such a system, the temperature was

very dependent upon the thermodynamic properties of the fuel. For example, a $\pm 5\%$ change in the gas phase heat capacity of the fuel caused a $\pm 7\text{K}$ change in the calculated mixture temperature.

First, the feasibility of the experimental technique will be demonstrated by studying iso-octane, a fuel for which the thermodynamic properties are well known. Second, the data for iso-octane will be used as a standard for determining any non-adiabatic behavior of the apparatus. Finally, Jet-A will be studied under identical conditions.

Results and Discussion

The initial data were taken with iso-octane and fuel injector A. Temperatures of fuel/nitrogen mixtures were measured for different amounts of fuel injected into the hot nitrogen stream. These measurements were compared to the temperatures calculated by the chemical equilibrium program for 298K liquid fuel and 800K nitrogen. Since the experimental fuel and nitrogen temperatures could not be maintained at exactly these conditions, small corrections were required to reduce these to the same starting conditions. The data for iso-octane are shown in Figure 2. It was observed that for low fuel mole fractions the experimental temperatures were below the calculated ones. This behavior is expected when the experimental apparatus is not adiabatic. However, at higher fuel mole fractions, the measured temperatures were much higher than the calculated ones and tended to level off. This suggests that complete vaporization had not been obtained at the monitoring station 68 cm downstream of the point of fuel injection. In discussions with Ingebo (10), it was suggested that vaporization could be improved by increasing the gas velocity and providing a constant area section to account for the stream break-up distance (about 2.5 cm). Injector A was modified by attaching a 3.0 cm addition at the inlet of each nozzle, as shown in Figure 1b. The calculated drop size obtained with the modified fuel injector is about $22\text{ }\mu\text{m}$. With the previous design, calculated fuel drops were about $44\text{ }\mu\text{m}$ at the throat of the nozzles, but droplets 2.5 times larger were calculated at a distance 2.5 cm downstream of the throat. These modifications should significantly improve vaporization.

Fuel injector B proved to be very successful, as shown by the iso-octane data in Figure 3. All the experimentally measured temperatures were below the calculated curve and the data showed a similar shape. This suggests that vaporization was complete. The temperature difference can be attributed to apparatus heat losses. These heat losses increase as the mixture temperature increases, which is the behavior expected for a non-adiabatic system. A curve fit to the experimental data indicated a heat loss varying from 7 degrees at 460K to 23 degrees at 580K. The system was calibrated by plotting the difference between this curve and the calculation as a function of temperature.

The measured temperatures for Jet-A/nitrogen mixtures are shown in Figure 4a. The behavior is exactly that observed for the iso-octane data. Correcting the experimental data points for

the heat losses from the calibration curve produced the results shown in Figure 4b. These data are in excellent agreement with the temperatures calculated using the coefficients derived from the thermodynamic data for Jet-A.

The extent of vaporization of a fuel with an end boiling point of 532K (4) was checked by using the Clapeyron equation which relates the boiling temperature (T) of a liquid with its vapor pressure (P),

$$\ln P = A + B/T \quad 4)$$

Data of vapor pressure reported in reference 4 were used to determine the constants A and B. The line obtained from the equation is shown in Figure 5. The region under the line (region I) corresponds to only vapor present, and the region above the line (region II) corresponds to liquid and vapor. Data points for the experimentally measured temperatures and partial pressures fall in region I, indicating complete vaporization of the fuel.

CONCLUSIONS

An experimental technique has been described in which the temperatures of very rich fuel/nitrogen mixtures were measured. These temperatures were shown to be dependent on the thermodynamic properties of the fuel. Iso-octane was used to test the feasibility of the technique and to calibrate the apparatus for heat losses. Coefficients were derived from thermodynamic data so that a Jet-A fuel could be included in the NASA Lewis chemical equilibrium program. The experimental data obtained for Jet-A in our calibrated apparatus were in excellent agreement with the calculated temperatures, confirming the correctness of the coefficients for the polynomials used in the program. This experimental technique is an excellent tool for verifying the thermodynamic properties of any multi-component fuel.

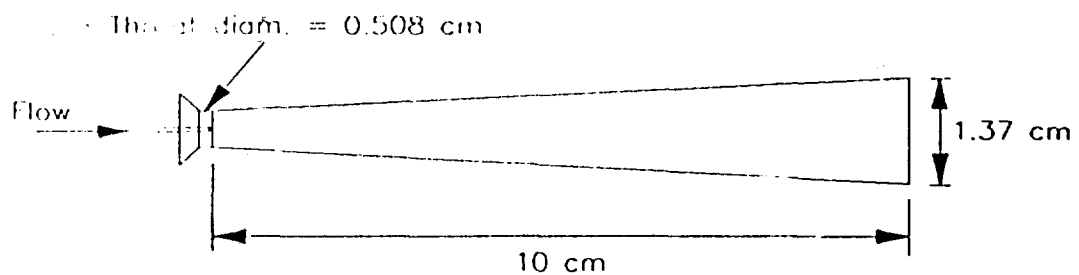
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Figure 1 - Fuel Injectors

a) Fuel Injector A



b) Fuel Injector B

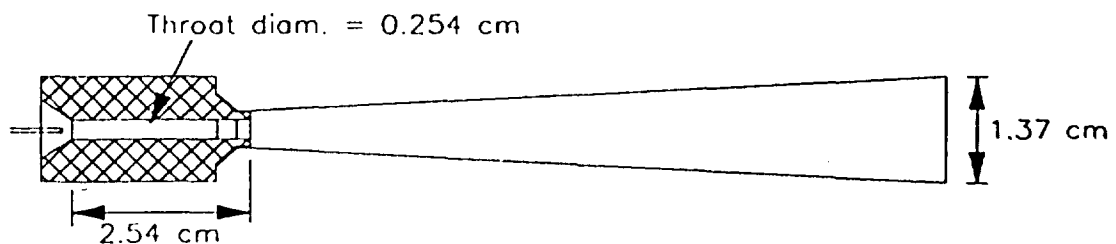


Figure 2 – Experimental Data for Iso-Octane (Fuel Injector A)

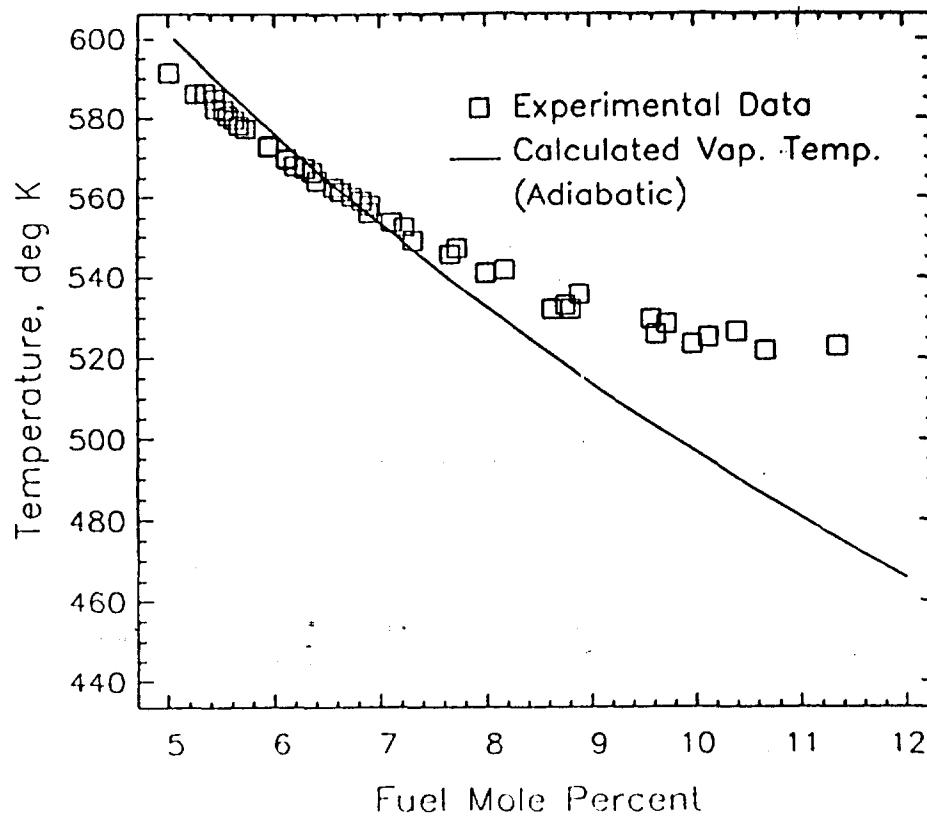


Figure 3 – Experimental Data for Iso-Octane (Fuel Injector B)

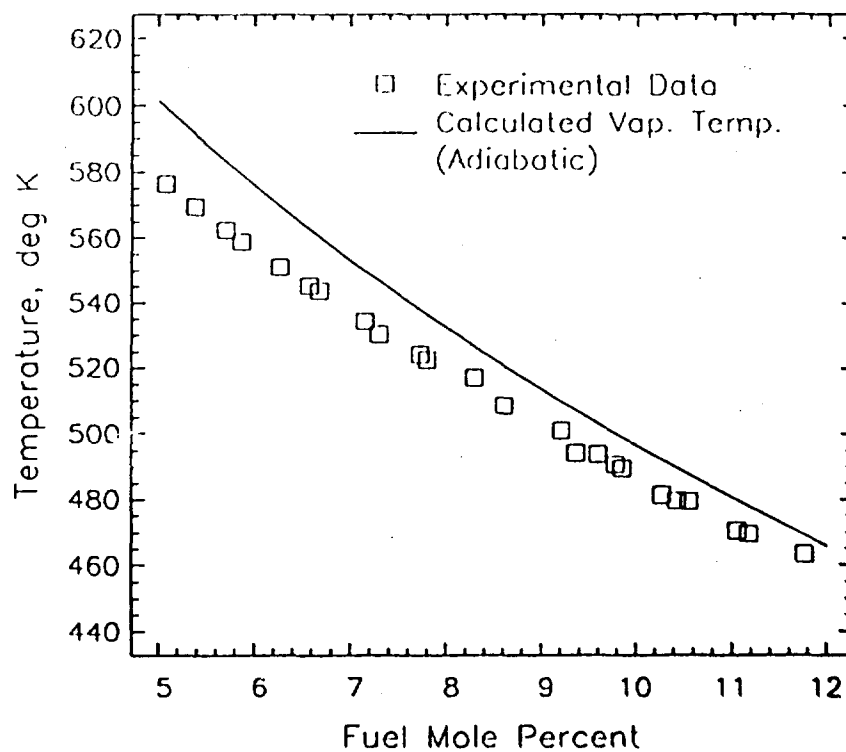


Figure 4 – Experimental Data for Jet-A (Fuel Injector B)

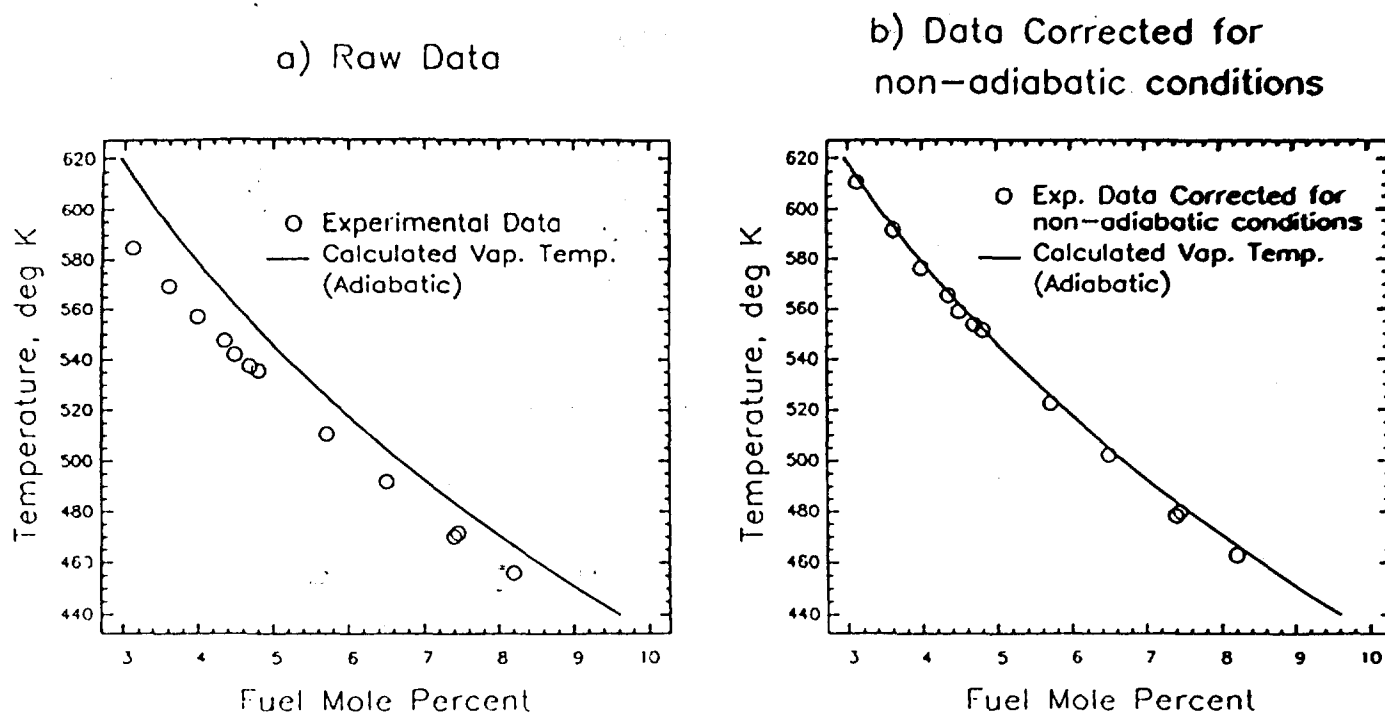
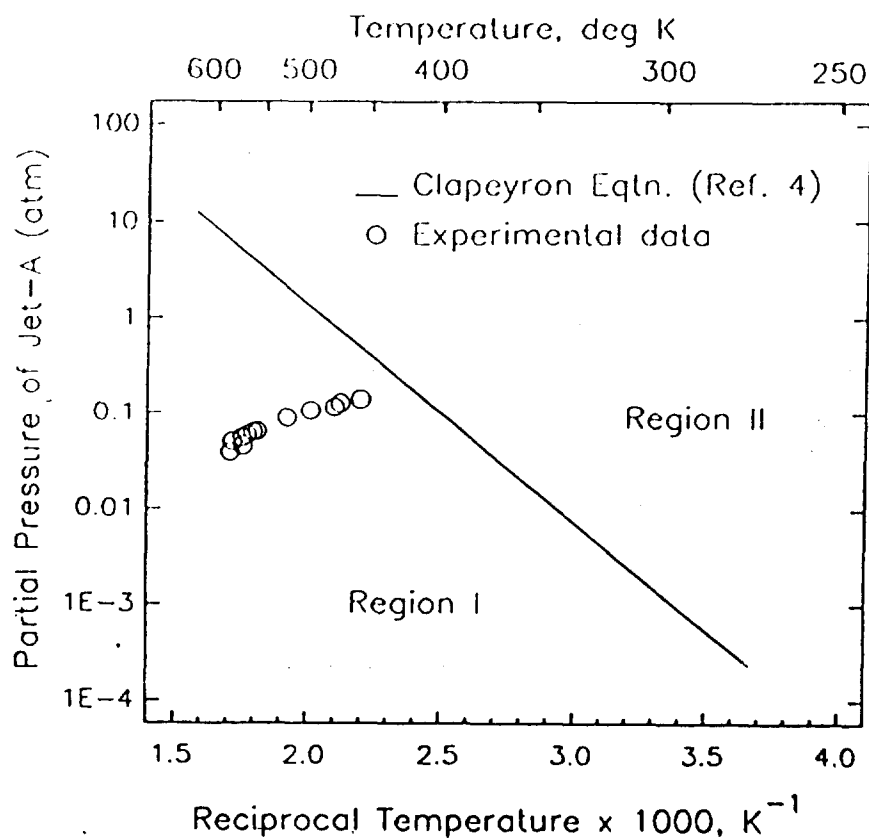


Figure 5 – Vaporization Temperature for Jet-A



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