A Step Towards CO₂-Neutral Aviation

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ABSTRACT

An approximation method for evaluation of the caloric equations used in combustion chemistry simulations is described. The method is applied to generate the equations of specific heat, static enthalpy, and Gibb's free energy for fuel mixtures of interest to gas turbine engine manufacturers. Liquid-phase fuel properties are also derived. The fuels include JP-8, synthetic fuel, and two fuel blends consisting of a mixture of JP-8 and synthetic fuel. The complete set of fuel property equations for both phases are implemented into a computational fluid dynamics (CFD) flow solver database, and multi-phase, reacting flow simulations of a well-tested liquid-fueled combustor are performed. The simulations are a first step in understanding combustion system performance and operational issues when using alternate fuels, at practical engine operating conditions.

INTRODUCTION

Major issues confronting today's aviation community center on fueling supply and not so much on emissions per se, but on climatic change and the potential for extinction engendering a significant effort to neutralize anthropogenic effects. Realizing that small changes in one area of the planet can make large differences in climatic conditions in other areas (planetary telekinesis¹), the aviation industry is diligently seeking alternate fueling and combustion methodology to mitigate harmful emissions and become CO₂ neutral. Alternate liquid fuels as derived from coal (CTL) or natural gas (GTL), termed "synfuels," when refined as aviation fuels and combusted, still release significant amounts of CO_2 , water, and hydrocarbons but less than Jet-A. Other plant-derived fuels, termed "biofuels," depend heavily on currently available food crops such as rice, wheat, corn, and soybeans, yet other forms such as switchgrass, algae, halophytes, palm oil, and similar cellulose or oil plant feedstocks, could become effective future fueling feedstock sources. Potentially biofuels could, through carbon trade-off, provide a way for aviation to partially achieve a goal of becoming CO_2 neutral while still using "drop-in" fuels for legacy aircraft. Currently, synfuels and blends are moving through the certification process.

Understanding combustor design and performance issues using alternate fueling is a step toward understanding aviation impact on climatic change and energy independence. In this paper we baseline combustor performance to the trapped vortex combustor (TVC) with cavity-only fueling using Jet-A fuel to simulate the experimentally fueled JP8+100 TVC. This computationally (with a computational fluid dynamics (CFD) flow solver) and experimentally established baseline is then compared to that computed using two other fueling methods, syn-fuel and JP-8 fuel. Thermophysical properties for these fuels are not yet available from the National Institute of Standards and Technology (NIST), and a method to simulate the needed combustor parameters for these fuels is synthesized and discussed.

The 10-component simulation volume fraction of syn-fuel is based on the major constituents of a synthetic manufactured fuel supplied to the U.S. Air Force Research Laboratory at Wright-Patterson Air Force Base

¹Planetary interactions happening in one place, affect other places seemingly without any connection (Flannery, 2006).

(AFRL/WPAFB). In the lower temperature regime, thermophysical properties of the 10 components are derived from the NIST code SUPERTRAPP (STRAPP) (Huber (2007)). In the higher temperature regime the properties are derived using a simple Cp⁰/R relation based on the McBride-Gordon NASA thermodynamic code (McBride et al., 2002). The 12-component JP–8 fuel is simulated in a similar manner. For combustor computations, each multicomponent mixture is simulated as a homogeneous fluid.

Based on this chemical mixture information, this work presents CFD-generated TVC cavity-only fueling performance for the following fueling cases:

- 1. Liquid JP–8 fuel with gaseous JP–8 fuel real gas properties.
- 2. Liquid Synthetic fuel with gaseous synthetic fuel real gas properties.
- 3. Liquid JP-8 50/synthetic 50 fuel with associated real gas properties.
- 4. Liquid JP–8 70/synthetic 30 fuel with associated real gas properties.

These fuels and blends were chosen to reflect current and projected fuels used for aviation, and those fuels available for experimentation including AFRL B52 flight tests. Also, prior testing found JP8+100 and Jet-A to have similar TVC combustion characteristics (Hendricks et al., 2001). In interpreting the TVC combustor simulation results, emphasis is placed on combustor quantities of engineering interest, such as spray droplet patterns, combustor flame patterns, and combustor exit plane quantities.

ANALYSIS METHODS

DETERMINATION OF THERMOPHYSICAL PROPERTIES OF ADVANCED, GASEOUS FUELS -McBride et al. (2002) established the renowned thermophysical properties code that is the standard for combustion. This code has coefficients for Jet-A, JP–10 and 2000 other species and components tabulated in

appendix D of NASA/TP-2002-211556, so $C_p^0(T)/R$

and other caloric properties can readily be determined. Gracia-Salcedo et al. (1988) have shown that 2,2,4trimethylpentane (isooctane) [224TMP] is a very good caloric simulant for Jet-A and is available in both McBride et al. (2002) and STRAPP (Huber, 2007).

Fuel simulations for JP–8 are given by Heneghan et al. (1993), and those for synthetic fuels by Corporan et al. (2005), Edwards and Murice (2001), and Edwards et al. (2004). An often-used assumption is that JP8+100 is similar in mixture to JP–8 simulant and that Syntroleum fuels are similar in composition to synthetic fuel given by Corporan et al. (2005). Discussions with Tim Edwards (2006, AFRL/WPAFB) indicated that Syntroleum fuel could be characterized as n-duodecane (C12).

The NIST computer program NIST4, also called SUPERTRAPP (STRAPP), characterizes fluid mixtures and was developed principally for the hydrocarbon liquid fuels industry. A recent release contains many of the components found in JP–8 or Syntroleum fuels, and also exotetrahydrodicyclopentadiene (JP–10).

ANALYTICAL PROCEDURE - McBride's caloric equations for $C_p^0(T)/R$ form the basis for determining a simplified formulation of caloric properties. McBride provides the form-similar equations for caloric properties:

$$C_{p}^{0}(T)/R = a_{1} T^{-2} + a_{2} T^{-1} + a_{3} + a_{4}T + a_{5}T^{2} + a_{6}T^{3} + a_{7}T^{4}$$
(1)

$$H^{0}(T)/RT = -a_{1}T^{-2} + a_{2}\ln T/T + a_{3} + a_{4}T/2$$

$$\cdot a_5 T^2 / 3 + a_6 T^3 / 4 + a_7 T^4 / 5 + b_1 / T \qquad (2)$$

$$S^{0}(T)/R = -a_{1}T^{-2}/2 - a_{2}T^{-1} + a_{3}\ln T + a_{4}T +a_{5}T^{2}/2 + a_{6}T^{3}/3 + a_{7}T^{4}/4 + b_{2}$$
(3)

From the fundamentals of thermodynamics, Gibbs free energy and mixture internal energy are computed, respectively, as

$$G^{0}(T)/RT = [H^{0}(T) - TS^{0}(T)]/RT = H^{0}(T)/RT - S^{0}(T)/R$$
(4)

and

$$U^{0}(T)/RT \approx H^{0}(T)/RT$$
 (5)

where

$$T^{-1} \int [C_p^0(T)/RT] dT = H^0(T)/RT$$
 (6)

and

$$\int [C_p^0(T)/RT] dT = S^0(T)/R$$
 (7)

In these equations, C_{ρ}^{0} is the mixture specific heat, H^{0} is the mixture static enthalpy, S^{0} is the mixture static entropy, G^{0} is the mixture Gibbs free energy, and U^{0} is the mixture internal energy.

The first set of comparisons were made using McBride's Jet-A coefficients and the $C_p^0(T)/R$ values from the NIST STRAPP code with JP–8 simulant, C12 and 224TMP for the range 300 to 1000 K at a pressure of 0.0001 MPa, shown in Figure 1. While having different values for a given *T*, the similarities were striking. Subsequent investigation of the $H^0(T)/RT$ and $S^0(T)/R$ values revealed the same form similarities.



Figure 1. Similarities of the $C_p^0(T)/R$ for four fuels: two mixtures, JP–8 and Jet-A, and two pure components, n-duodecane (C12) and 2,2,4-trimethylpentane (224TMP).

These similarities prompted an investigation into the nature of a technique to extrapolate $C_p^0(T)/R$ beyond STRAPP's temperature range to that necessary for combustion computations. A simplified technique revealed that McBride's Jet-A $C_p^0(T)/R$ value away from the saturation boundaries could be approximated with the form

$$C_p^0(T)/R = AT^{(-1/2)} + B$$
 (8)

$$H^{0}(T)/RT = 2AT^{(-1/2)} + B + C_{1}/T$$
(9)

$$S^{0}(T)/R = -2AT^{(-1/2)} + B \ln T + C_{2}$$
(10)

(11)

and Gibb's free energy:

$$G^{0}(T)/RT = [H^{0}(T) - TS^{0}(T)]/RT$$
$$= H^{0}(T)/RT - S^{0}(T)/R$$

In these expressions, the constants C_1 and C_2 are determined by first setting the particular constant (e.g., C_1 for $H^0(T)/RT$) to 0 and determining the matching reference value $H^0(T)_{ref}/RT_{ref}$ or $S^0(T)_{ref}/R$ from those generated by STRAPP or McBride's code depending on the source of the data to be used in the comparison.

$$C_{1} = \{T[H^{0}(T)/RT]_{\text{STRAPP}} - [H^{0}(T)/RT]_{\text{C1}=0}\}_{T=Tref}$$
(12)

$$C_2 = \{ [S^0(T)/R]_{\text{STRAPP}} - [S^0(T)/R]_{C2=0} \}_{T=Tref}$$
(13)

 $T_{\rm ref}$ was either 300 K or 400 K, with the latter providing better overall agreement and usually sufficiently far away from the saturation boundaries.

The liquid phase properties required for these fuels were determined analytically as well. Of importance to liquid fuel injection, the properties determined included density, specific heat, heat of vaporization, and thermal conductivity. These properties were implemented into the CFD flow solver database in order to simulate the droplet dynamics and evaporation characteristics accurately (described in forthcoming sections).

SIMPLIFIED FORM EXTRAPOLATIONS -This simplified form (Eq. (8)) permits extrapolation to elevated temperatures and using the Jet-A $C_p^0(T)/R$, and McBride's equations the constants A and B were determined and the results were compared with the actual $C^0_p(T)/R$ for Jet-A (McBride's equations) over the range of 300 to 3000 K. The values compared favorably, with a reasonable engineering accuracy of better than 5% over the 400 to 3000 K temperature range. However, departures of 20% to 30% deviation occur near 300 K, which is close to or on liquid-vapor boundaries. Above 3000 K the deviations continue to fall nearly linearly to 7.5% at 6000 K, reflecting the inaccuracies in $C_p^0(T)/R$ reproducing the calculated using the equations of McBride's code. Better agreement between the extrapolated method and McBride's code predictions is found in the integrated properties, such as $S^{0}(T)/R$, which for the most part is within about 1% as shown in Figure 2. The deviations in $H^{0}(T)/RT$ depend on where the locus changes from negative to positive, where small deviations make large differences. Generally the $H^{0}(T)/RT$ is within 3%. Perhaps a better way to illustrate the deviations would be to add a constant to ensure all values are positive, as is the case with $S^{0}(T)/R$.

It was also found that much better overall agreement could be generated if the $C_{\rho}^{0}(T)/R$ were fitted over the range 400 to 3000 K when using data from STRAPP at the lower temperatures. This establishes a methodology to extend $C_{\rho}^{0}(T)/R$, caloric properties in general, over the range 300 to 3000 K with reasonable engineering confidence.



Figure 2. Deviations in $S^0(T)/R$ calculated by approximate extrapolation method to those calculated based on equations from McBride's code.

STRAPP—APPROXIMATE **MCBRIDE** CODE COMPARISONS - To illustrate that the technique applies to STRAPP-generated data, McBride's code also coefficients for the pure component fluid has exotetrahydrodicyclopentadiene (JP-10). Generating the

 $C_{p}^{0}(T)/R$, $H^{0}(T)/RT$, and $S^{0}(T)/R$ from McBride's method

over the range 300 to 3000 K provides the basis for comparison. Using STRAPP input for JP-10, these same values were generated using the approximate extrapolation technique over the range 300 to 1000 K. The values are similar to those found for Jet-A. Using the extrapolation for the range 1000 to 3000 K found similar agreement, thus establishing the technique linking the properties generated by STRAPP with those generated by McBride's code, and it provides reasonable engineering confidence in the caloric computations for mixtures as generated by STRAPP and extrapolated to higher temperatures (Fig. 3).

With these comparisons it was then assumed that fluid mixtures characterized by STRAPP in the lower temperature ranges could, through a suitable fit to these data using the simplified method, be extrapolated with engineering certainty to reasonable elevated temperatures in order to characterize combustion. The $Cp^{\circ}(T)/R$ and $H^{\circ}(T)/RT$ values are important parameters in determining combustion temperature.

The components, volume, and mass fractions used to simulate JP-8 and synthetic fuels are given in Tables 1 and 2, respectively. Blended fuel properties were derived

using a mole-fraction weighting procedure. The carbonto-hydrogen ratios (C/H), molecular weights (MW), and approximate extrapolation method coefficients for each fuel are listed in Table 3. The C/H values were determined from the mole fraction product of the C/H component chemical composition summed over mixture components. In all cases, homogeneous singlecomponent simulations of multicomponent fluid mixtures are used in the combustor simulations, including both liquid phase and gas phase.



Figure 3. Comparison between approximate extrapolation methods for $C_p^0(T)/R$ for fluid exotetrahydrodicyclopentadiene (JP-10).

Table 1. JP–8 simulant components and fractions used as input to STRAPP (Heneghan et al., 1993)						
JP–8 component	Mass	Mole	Molecular	Mass/weight		
		fraction	fraction	weight		
2,2,4-trimethylpentane						
(isooctane)	224TMP	0.0500	0.0640	114.22	0.000437752	
Methylcyclohexane	MCC6	0.0500	0.0745	98.19	0.000509217	
meta-xylene	MXYL	0.0500	0.0688	106.17	0.000470943	
Cyclooctane	CC8	0.0500	0.0652	112.22	0.000445553	
n-decane	C10	0.1500	0.1542	142.28	0.001054259	
Butylbenzene	C4BNZ	0.0500	0.0545	134.22	0.000372523	
1,2,4,5-tetramethylbenzene	1245TMBNZ	0.0500	0.0652	112.2	0.000445633	
1,2,3,4-tetrahydronaphthalene (tetralin)	TETRALIN	0.0500	0.0553	132.2	0.000378215	
n-dodecane	C12	0.2000	0.1717	170.34	0.001174122	
1-methylnaphthalene	1MNAPH	0.0500	0.0514	142.2	0.000351617	
n-tetradecane	C14	0.1500	0.1106	198.39	0.000756086	
n-hexadecane	C16	0.1000	0.0646	226.45	0.000441599	
Mixture		1.0000	1.0000	^a 146.25 ^b 146.25	0.006837519	
STRAPP				147.8		
a) / alive la a a a la a se a a a fue atien						

Value based on mass fraction.

^bValue based on mole fraction.

Table 2.	Syntroleum	simulant	components	and fractions	used as	input to	STRAPP
	-	(Corporan et	al., 2005).			

Syntroleum component		Mass	Mole	Molecular	Mass/weight
		fraction	fraction	weight	
n-octane	C8	0.0430	0.0570	114.22	0.000376466
n-nonane	C9	0.1000	0.1181	128.26	0.000779666
n-decane	C10	0.1870	0.1990	142.28	0.00131431
n-undecane	C11	0.1900	0.1841	156.31	0.001215533
n-dodecane	C12	0.1320	0.1174	170.34	0.000774921
n-tridecane	C13	0.0930	0.0764	184.36	0.000504448
n-tetracecane	C14	0.0740	0.0565	198.39	0.000373003
n-pentadecane	C15	0.0270	0.0192	212.42	0.000127107
3-methyloctane	3MO	0.0720	0.0850	128.26	0.00056136
2-methylnonane	2MN	0.0820	0.0873	142.29	0.000576288
Mixture		1.0000	1.0000	^a 151.44 ^b 151.44	0.006603101
STRAPP				151.4	

^aValue based on mass fraction.

^bValue based on mole fraction.

Table 3. Carbon-to-hydrogen ratios (C/H), molecular weights (MW), and curve
fit coefficients from Equations (8) through (10) used in the approximate
extrapolation method for the four fuels investigated.

Fuel	Coeffic	Coefficients for Approximate Extrapolation Method				
	C/H	MW	A	В	<i>C</i> ₁	<i>C</i> ₂
JP-8	10.605/20.15	147.83	-1542.6	110.9	-314.83	-746.54
JP-8 (70)/syn (30)	103629/21.72	148.94	-1582.4	113.9	-2321.47	-763.57
JP–8 (50)/syn (50)	10.620/21.09	149.60	-1607.3	115.8	-3673.2	-775.93
Synthetic	10.653/23.306	151.40	-1671.8	120.68	-6983.8	-808.36

Table 4. Liquid phase fuel properties for the four fuels investigated.

Fuel	Liquid-Phase Fuel Properties ^a				
	Molecular	Boiling point	Density	Density at	Latent heat,
	weight	at 0.1 MPa,	at 298 K,	boiling point, ^b	kJ/kg
		K	kg/m ³	kg/m ³	
JP-8	147.83	436.3	800.7	681.7	255.0
JP–8 (70)/syn (30)	148.94	439.6	783.6	660.5	287.0
JP–8 (50)/syn (50)	149.6	441.7	772.8	647.0	296.0
Synthetic	151.4	447.2	747.0	614.6	290.0

^alsothermal flash property.

^bOne or two components may be in solid phase.

Liquid phase fuel properties were required for the initial injection of liquid-fuel spray droplets into the combustor through orifice injectors. These were derived using a mole-fraction weighting procedure. Key liquid property values are indicated in Table 4, including liquid molecular weight, boiling point at 0.1 MPa, density, and latent heat of vaporization. Additional property values required for accurate spray droplet dynamics and evaporation rates include specific heat, viscosity, and thermal conductivity, which were also determined as part of this effort.

TRAPPED VORTEX COMBUSTOR (TVC) EXPERIMENTAL RIG - The trapped vortex combustor (TVC) sector rig at the Air Force Research Laboratory, Wright-Patterson Air Force Base is used as the experimental basis. It is a combustor geometry for which there exists a wealth of validation data including, for example, wall pressures, emissions, and high-frame-rate video for flame structure. The inlet diffuser and combustor geometry are accurately characterized in CAD, with known coolant flows and spray droplet characterizations. The TVC operates stably over a wide range of equivalence ratios and pressures and has been useful in studies of altitude restart and lean blow out (LBO) (Hendricks et al., 2001 and 2004). A schematic of the test rig is shown in Figure 4, which illustrates the airflow and fuel injection sites as well as the general flow patterns expected in the combustor.



Figure 4. (a) Schematic diagram of the trapped vortex combustor. Arrows indicate the major flow components. Liquid fuel is injected into the TVC cavity and also directly into the main combustor through orifices in the diffuser. In the present study, cavity-only fuel injectors are utilized. (b) Test rig hardware for the trapped vortex combustor, with near sidewall removed for optical access. The photograph shows 10 fuel injector modules in the spanwise direction

Provision for addition of water mist for pollutant emission reduction studies is also indicated. A photograph of the combustor hardware is shown in Figure 4, with the sidewall removed for optical access. Components of the rig include the tripass diffuser, combustor bulkhead, heat shield, and combustor duct that exhausts to a vent. Combustor walls are cooled through effusion holes along the entire interior wall, and film cooling through slots along the combustor upper and lower walls.

Engine compressor exit air is emulated by a plenum, and is connected to the TVC combustor through a tripass diffuser. This diffuser configuration splits the flow evenly, with the upper and lower diffuser flow paths providing high-speed shear layers that drive the cavity flows and entrain products of combustion into the main flow.

The center diffuser flow path provides a high-speed jet that interacts with the outer diffuser flows and further mixes the products as the flow approaches the combustor exit. The result is a stable combustion process with high efficiency, within a compact configuration. The TVC combustor is fueled in two different ways. Liquid fuel is injected through simple orifice injectors into the main diffuser flow paths, with the high-speed crossflow atomizing the liquid fuel jet into a fine mist. Independently, liquid fuel is injected into the TVC cavities through simple orifice injectors. The cavity spray droplets are injected into a hot, reacting flow environment and evaporate rapidly. Using this experimental rig, and through a combination of cavityonly, cavity and main, and main-only fueling schemes, different operating conditions can be produced in the rig, allowing for investigation of a wide variety of flow phenomena in the experiment.

The effect of the spray droplet injection conditions on the combustor flow field and combustor exit pattern factor has been investigated previously (Hendricks et al., 2004). During that effort, the initial droplet size distributions were determined for the engine operating conditions used in this investigation. For the main injector, and for a nominal plenum pressure of 50 psia (344.6 kPa), the Rosin-Rammler droplet size distribution was $R_{32,10} = 3 \mu m$, $R_{32,50} = 6 \mu m$, and $R_{32,90} = 12 \mu m$. For the cavity injector, the Rosin-Rammler droplet size distribution was $R_{32,10} = 5 \mu m$, $R_{32,50} = 8 \mu m$, and $R_{32,90} = 10 \mu m$. The effects of water misting and water injection through the orifice injectors were also studied (Brankovic et al., 2005), showing computationally the potential benefits of water addition to reduction of NOx at the combustor exit.

Both of those parametric studies above showed the significant variation in combustor exit parameters (average temperature, combustion efficiency, and flame structure and pattern factor) due to even small upstream differences in liquid fuel droplet size and fuel water vapor content.

In the present parametric study, therefore, the droplet size distribution and overall and cavity-based equivalence ratio are held constant; only the fuels are varied to isolate the effects of the differences in the liquid and gaseous properties. Cavity equivalence ratio for each case is $\phi_{cav} = 2.2$, while the overall equivalence ratio (entire combustor including all combustion, driving and cooling flows) is $\phi_{overall} = 0.53$.

COMPUTATIONAL FLUID DYNAMICS SIMULATIONS USING ALTERNATE FUELS - To characterize the performance of the various fuels in the TVC test rig, a

suite of computational fluid dynamic (CFD) simulations are performed. The four fuels investigated include JP-8, synthetic, and blended fuels consisting of JP-8 (50%)/synthetic (50%) and JP-8 (70%)/synthetic (30%). All corresponding liquid fuel and gaseous fuel properties have been derived and installed in the flow solver property database. Combustion chemistry is modeled using the three-step reduced chemistry model of Molar and Marek (2003), which consists of a fuel breakup and oxidation equation into CO and H₂O (Step 1), oxidation of CO into CO₂ (Step 2), and dissociation of N_2 and O_2 into NOx (Step 3). Previous validation studies (Brankovic et al., 2005; Hendricks et al., 2001 and 2004) provide useful information on injection conditions for the liquid fuel, including droplet diameter distributions, velocities, and spray cone angles.

The test rig geometry is accurately represented in the form of a computer-aided design (CAD) solid model. Using the CAD model, all boundary conditions are tagged, including all major inflows, secondary flows, and film cooling slots. Following this, the volume is discretized using an unstructured mesh generator. The model is exported, and the domain is decomposed and load balanced for running on parallel networked computers for rapid turnaround time. Results are post-processed graphically and quantitatively using a mass-averaging algorithm.

RESULTS OF FLOW SIMULATIONS - The basis for comparison of the combustor simulations is inspection of the computed flame structure at the TVC midplane and computed mass-average quantities at the combustor exit. Comparison of the flame structure for the four different fuels is shown in Figure 5. The contours shown are each taken at the combustor midplane, using the same temperature scale, allowing direct comparison. Clearly, the flow structure is similar, nearly identical, for each fuel. Upon inspection of the fuel properties, both liquid and gaseous, this is not unexpected. The flow structure similarity suggests that droplet evaporation and dynamics patterns are nearly identical, resulting in the similar burning patterns. Each of the combustor simulations exhibits a centrally peaked temperature profile at the flow exit. The effects of multicomponent spray modeling are yet to be determined.

Carbon monoxide generation and flow pattern is shown in Figure 6 for the four cases. Rapid formation of CO in the TVC cavities is observed for each case. As the cavity flow is entrained by the diffuser flow and further heated within the combustor, the CO oxidizes into CO_2 ; this oxidation process is observed in the CO_2 contours shown in Figure 7, again for each of the four fuels.

Combustor exit quantities are provided in Table 5. The values were obtained by mass averaging the computed flow field at the combustor exit. Temperatures vary by about 24 K (or about 1.5% max to min) at that location. Thus, despite strong similarities in computed flow structure, this temperature difference produced by these fuels is potentially enough to require alterations in the cooling scheme for the turbine first vane in a practical application. An inspection of the tabulated values shows that the highest exit temperatures correspond to the least amount of unburned fuel at the exit. Likewise. lowest exit temperatures correspond to greatest amounts of unburned fuel. The minor differences occurring upstream in the cavities and combustor are apparently enough to cause significant differences in the engineering quantities sampled at the combustor exit.



Figure 5. Combustor midplane contours of static temperature, for the labeled fuels. Flame structure is strikingly similar in all cases.



Figure 6. Combustor midplane contours of carbon monoxide (CO) mass fraction. Strong peaks occur within the high residence time cavities; with increased time and temperature, the majority of CO oxidizes to CO_2 as the flow reaches the combustor exit plane.



Figure 7. Combustor mid-plane contours of carbon dioxide (CO_2) mass fraction. A characteristic CO_2 formation pattern is observed in each case, with strong centrally oriented peaks occurring as flow exits the combustor.

 Table 5. Computed combustor exhaust plane quantities, showing strong similarity of the temperature and species concentrations among the different fuels

			<u> </u>	
Fuel	Mass-Averaged Combustor Exit Quantities			
	Temperature,	CO mass	CO ₂ mass	Unburned fuel
	K	fraction	fraction	mass fraction
JP–8	1600.0	0.00031	0.094	0.00049
JP–8 (70)/syn (30)	1622.9	0.00030	0.097	0.00042
JP–8 (50)/syn (50)	1624.1	0.00029	0.097	0.00042
Synthetic	1603.1	0.00039	0.096	0.00057



Figure 8. Frames from animation of CFD-simulated thermal flow field, shown in different orientations (temperature is in Kelvins). Arrows in figure (a) indicate flow directions. Solid particles, color coded by local gas temperature, are used to visualize the flow in the TVC cavity and combustor duct. Figure (a) is an isometric, mainly lateral view, with emphasis on the mixing region between diffuser, cavity and combustor flow. Figure (b) is similar to (a), but with different orientation. Figure (c) is a reversed isometric view, showing more of the combustor flow downstream. Figure (d) is an aft-looking forward view towards the orifice fuel injectors, showing some of the overall mixing pattern in the lengthwise direction.

The increase in CO and unburned hydrocarbon mass fractions, indicated in Table 5, is a relative measure of how these fuels respond within the tripass TVC combustor. Computations show that synfuel droplet sprays have longer residence times within the combustor relative to JP–8 or blended fuels. Moses (2006) shows "no effect" of CO or other emissions of synfuel relative to Jet-A; experimental TVC data are needed to resolve this issue. Emission signatures are important especially to the military cross-platform common fuels initiative.

In addition to these comparisons, the complex flow structure is studied in a three-dimensional sense using animations. A series of still images taken from an animation of the flow is shown in Figure 8. In each, the TVC combustor geometry is shown translucently, to view the inside of the flow. Particle paths are seeded at representative locations, such as upstream in the diffuser legs, inside the plenums with driving airflow, and inside the cavity itself. The particle paths trace out the gas phase flow and are colored by local gas phase static temperature. Numerous vortices are observed inside the driven cavity, and that flow is entrained by the diffuser leg flow. Some of the heated products of combustion are trapped along the inner combustor wall, between the center and outer diffuser legs. This serves as flameholder acting upon the center flow. Comparison of these results with high-frame-rate videos and long-timeaveraged still photos of the flow show good consistency in flame shape (Brankovic et al., 2005).

CONCLUSION

The simplified form of the gas phase caloric equations generated using the NIST STRAPP code, the NASA McBride code. and а systematic curve-fitting methodology, work within established well an computational fluid dynamics (CFD) flow solver. Upon further benchmarking, the actual code speed-up for combustion chemistry CFD cases in practical geometries will be quantified. Computed flow structure for the four fuels, using a trapped vortex combustor experimental rig as a test case, show strong similarities. This is true for the temperature as well as the CO and CO₂ mass fraction contours. Inspection of the mass-averaged combustor exit quantities, however, indicates that temperature

differences may be sufficient to require reconsideration of turbine fueling schemes. Experimental validation studies using these fuels, over a range of operating conditions, are expected.

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DEFINITIONS, ACRONYMS, ABBREVIATIONS

Α	constant in Eq. (8), K ^{1/2}
a ₁ , a ₂ , a ₃ , a ₄ , a ₅ , a ₆ , a ₇ B C C ₁ C ₂ C/H	Gordon-McBride constants constant in Eq. (8) carbon number constant in Eq. (9), K constant in Eq. (10) carbon-to-hydrogen ratio
$C_p^0(T)/R$	dimensionless specific heat
G ⁰ (T)/RT H ⁰ (T)/RT H MW R S ⁰ (T)/R T U ⁰ (T)/RT φ	dimensionless Gibbs free energy dimensionless enthalpy hydrogen number molecular weight universal gas constant (e.g., 8.314510 J/(mol-K) dimensionless entropy temperature, K dimensionless internal energy equivalence ratio
Subscripts: cav $C_1=0$ $C_2=0$ overall ref STRAPP	pertaining to cavity calculated with C_1 set to 0 calculated with C_2 set to 0 pertaining to entire combustor reference calculated by STRAPP code