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SCORES: Developing an Object-Oriented Rocket Propulsion Analysis Tool

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ABSTRACT

SCORES (SpaceCraft Object-oriented Rocket Engine Simulation) is an analysis tool being developed for conceptual-level spacecraft and launch vehicle design. Written in C++, SCORES provides rocket thrust and Isp for propulsion system trade studies. Common gateway interface scripts, written in Perl, provide an interface with the World Wide Web. The design parameters used in SCORES are mixture ratio, chamber pressure, throat area, and expansion ratio, making SCORES effective in multidisciplinary design optimization. This paper describes the current status in the development of SCORES, compares chemical equilibrium results against accepted equilibrium codes STANJAN and CEA, compares engine thrust and Isp predictions against available engine data for nine rocket engines, and discusses areas for future work. SCORES accurately predicts equilibrium mole fractions and adiabatic flame temperature over a wide range of operating conditions within 0.5%. Uncorrected errors of less than 10% within SCORES engine thrust and specific impulse calculations are within acceptable tolerances for use in conceptual-level design. Statistically correcting the performance predictions reduces these errors appreciably and provides the designer with additional information, the confidence interval of the calculations.

NOMENCLATURE

β	multiplier
ε	nozzle area ratio (A_e/A_t)
γ	ratio of specific heats
λ_k	element potential (G/RT)
A	area (in^2)
c*	characteristic velocity
C_f	thrust coefficient
Cp	constant-pressure specific heat
G	Gibbs free energy
g_c	unit conversion factor
g_j	(G/RT) for species *i*
h	specific enthalpy
Isp	specific impulse (sec)
$\dot{m}$	mass flow rate (lb./sec)
MW	molecular weight (kg/kg-mole)
N_i	moles of species *i*
$\mathbf{n}_{kj}$	element *k* atoms in species *j*
O/F	oxidizer to fuel ratio
p	pressure (psia)
R	gas constant
s	specific entropy
T	temperature (K)
x_j	mole fraction of species *i*

Subscripts

a	atmospheric
act	actual value
c	combustion chamber
calc	calculated value
e	nozzle exit

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M	perfect gas mixture
t	nozzle throat
thr	thrust

INTRODUCTION

SCORES (SpaceCraft Object-oriented Rocket Engine Simulation) is an analysis tool being developed for conceptual-level spacecraft and launch vehicle design to provide rocket thrust and Isp. SCORES, written entirely in C++, takes advantage of the language's object-oriented features to provide a code which is easily adapted to the user's needs. CGI (Common Gateway Interface) scripts, written in Perl, provide the wrapping agents needed to interface the C++ executable with HTML (HyperText Mark-up Language) web pages.

The motivation for developing this tool is to provide the conceptual-level spacecraft and launch vehicle designer with a tool capable of providing "quick-look" answers to propulsion system trade studies. Of importance in performing these trade studies is maintaining the appropriate level of fidelity. Therefore, the design parameters used in SCORES are top-level propulsion parameters that affect the overall vehicle design (mixture ratio, chamber pressure, throat area, and expansion ratio). This feature allows the designer to use SCORES effectively in an MDO (Multidisciplinary Design Optimization) environment. MDO brings together several disciplines and seeks optimal solutions to design problems with respect to the given design objective criteria. This paper describes the current status in the development of SCORES, compares results against accepted codes, and discusses areas for future work.

ANALYSIS PROCESS

SCORES determines rocket engine performance given nozzle expansion ratio (ε), throat area (A_t), chamber pressure (P_c), and mixture ratio (O/F). Engine performance prediction includes rocket thrust and Isp through chemical equilibrium, isentropic expansion, and statistical calculations.

First, equilibrium calculations provide the combustion product thermodynamic properties. Once the ratio of specific heats (γ), temperature (T), and molecular weight (MW) of the exhaust gasses are known, subroutines determine ideal nozzle performance in terms of thrust coefficient (Cf), characteristic exhaust velocity (c*), and mass flow rate ($\dot{m}$). These subroutines utilize expressions for frozen one-dimensional, isentropic expansion. Anderson[1] defines frozen flow as a flow where the reaction rates are precisely zero. The consequence of this assumption is to maintain a chemical composition constant, or frozen. This is the opposite of equilibrium flow, which implies infinitely fast reactions. Finally, a statistical sampling process corrects for variations in performance due to real processes and provides indications of thrust and Isp uncertainty.

Chemical Equilibrium:

Chemical equilibrium calculations provide exhaust gas thermodynamic properties. The method of element potentials, described by Reynolds[2], determines the mole fractions of the desired product species given O/F ratio and P_c. The observation that, at equilibrium, each atom of each element contributes exactly the same amount to the Gibbs free energy of each species, forms the basis for the method of element potentials. That amount of energy, the element potential, can be shown to be the eigenvalues, λ_k, of the following expression:

$$x_j = \exp\left(-\tilde{g}_j + \sum_{k=1}^{A} \lambda_k n_{kj} \right) \qquad \mathbf{(1)}$$

In the above expression, the index's j and k refer to the molecular species and atomic element respectively, where A is the number of elements. This expression, derived assuming a mixture of perfect gasses, allows the determination of any number of species mole fractions by solving for the unknown potentials of each element. This significantly reduces the number of unknown variables. Additionally, it can be shown that the Gibbs free energy obtains a minimum value at equilibrium[3]. The equilibrium problem can therefore be expressed formally as:

> *For a given temperature and pressure, minimize the Gibbs free energy of the product gasses, $G_{M,}$ subject to atom conservation.*

SCORES, as currently configured, only analyzes the combustion of liquid hydrogen, H_2, and liquid oxygen, O_2. Six product species are assumed: H_2O, H_2, O_2, H, O, and OH. Since there are only two unknowns, the hydrogen potential (λ_H) and the oxygen potential (λ_O), the design space is two-dimensional with each point (λ_H, λ_O) mapping to a unique set of mole fractions through the equation above. Each point thus relates to a unique G_M and mole ratio, N_H/N_O. SCORES uses a golden section search procedure on λ_O to minimize G_M. The golden section method, described in Vanderplaats[4], is an interval reduction procedure with a known convergence rate. At each λ_O, another golden section search is performed on λ_H to minimize the error between the actual and required, as defined by the O/F ratio, mole ratio. The mole fractions are used to determine the mixture MW and γ.

A secant method iteration, performed on temperature, minimizes the difference between the reactant and product enthalpies. This temperature defines the adiabatic flame temperature, which is assumed to be identical to the combustion temperature.

Table 1 Curve Fit Coefficients

	H2	***O2***	***H2O***	***H***	***O***	***OH***
α 0	3.933722685	5.057032641	2.746701247	0	2.116701865	3.82965272
α 1	0.059959468	0.019344927	30.60914939	1	0.05186064	1.03E-07
α 2	150.3903196	5.697101525	8.322294987	49.68	2.955440175	6.271142439
α 3	-0.004412135	-0.0079048	-0.002943495	0	-0.005555538	-0.004258877
α 4	12070.42761	-26.51339157	-10676.72408	0	-26.51339602	-23.59458512
α 5	-0.062041073	-0.022299194	-1.43295643	0	-0.222991108	-0.957671188
α 6	-148.3456013	3.134160952	-8.757141531	0	2.634767984	22.7425443
α 7	-0.004534063	-0.00055886	-0.001113711	0	-0.000658091	-7.95E-06
α 8	0.320522905	0.379109696	0.02592152	0.004953723	0.005042775	0.165010252
α 9	16472.49722	16597.84136	445.1886493	-0.459800415	-0.46970185	-5495.381807
α 10	2602.574292	2557.550016	19.01923983	-0.057167685	-0.095054963	5982.983104
α 11	-3.70E-05	-4.33E-05	-0.000505011	-0.018752263	-0.018913158	-2.15E-05
α 12	-19077.01074	-19157.52981	-466.4004923	-0.9925826	-1.042302694	-489.6674722
α 13	1.14E-05	1.36E-05	2.11E-05	-6.14E-06	-9.83E-10	6.06E-05
α 14	14.89646448	23.55885656	14.57864692	11.43447621	13.30284376	15.89591189
α 15	0.081547016	0.025063253	97.11760674	0.834978622	1.741901386	4.12E-06
α 16	127.8047615	7.283550034	-3.026749532	0.022134567	0.998014896	-7097.870774
α 17	-6.09E-05	-0.005651998	-0.010685824	-0.004795216	-0.002492277	-0.098017495
α 18	-584.850401	-26.51024332	-10676.72408	12502.30278	-0.541034286	-23.59458512
α 19	-0.000108893	-0.223380128	-1.43295643	-0.137602296	-0.015139915	-0.957671188
α 20	467.403068	4.836786448	-21.06978544	0.021642709	2.13815034	89.94157461
α 21	-0.000117769	-0.001055833	-0.00020979	-0.004614889	-0.000405464	6.19E-06

Thermodynamic Properties:

Curve-fit approximations to the Joint Army Navy Air Force (JANAF) thermochemical tables provide the thermodynamic data needed in the combustion calculations described above.

Because SCORES is written in an object-oriented language, the code can be written in self-contained units called classes. These classes can use the property of inheritance to access the data and functions contained within another class. The thermodynamic property class within SCORES makes use of this principle. A single base class contains the equations for the C_p, h, and s curve-fits while derived classes contain the specific values for the 22 coefficients for each of the individual species. The species classes also contain molecular weight and reference enthalpy. This object-oriented structure allows for the easy incorporation of additional species.

For simplicity, as well as to ensure smoothness everywhere, it was desirable to write one expression for the properties from 0 to 6000 K. The following equations provide the forms of the interpolating functions used:

$$\mathrm{Cp} = \alpha_0 + \log_{10}\left[\alpha_1(\mathrm{T}-1)\right] + \alpha_2 e^{\alpha_3 \mathrm{T}} + \alpha_4 e^{\alpha_5 \mathrm{T}} + \alpha_6 e^{\alpha_7 \mathrm{T}} \tag{2}$$

$$h = \alpha_8 + \alpha_9 \mathrm{T} + \alpha_{10} e^{\alpha_{11}\mathrm{T}} + \alpha_{12} e^{\alpha_{13}\mathrm{T}}$$

$$s = \alpha_{14} + \log_{10}\left[\alpha_{15}(\mathrm{T}-1)\right] + \alpha_{16} e^{\alpha_{17}\mathrm{T}} + \alpha_{18} e^{\alpha_{19}\mathrm{T}} + \alpha_{20} e^{\alpha_{21}\mathrm{T}}$$

Table 1 above lists the coefficients for each of the six species: H_2O, H_2, O_2, H, O, and OH. These values were obtained by minimizing the sum of the squares of the residuals between the predicted values and the JANAF table data.

Engine Performance:

Nozzle performance calculations utilize adiabatic flow relationships for a calorically perfect gas. A secant method iteration scheme determines the Mach number at the nozzle exit. Once exit flow conditions are known, the following ideal rocket equations generate classical engine performance parameters:

$$C_f = \sqrt{\frac{2\gamma^2}{\gamma-1}\left[\frac{2}{\gamma+1}\right]^{\frac{\gamma+1}{\gamma-1}}\left[1-\left(\frac{p_e}{p_c}\right)^{\frac{\gamma-1}{\gamma}}\right]} + \varepsilon\left[\frac{p_e - p_a}{p_c}\right] \tag{3}$$

$$\dot{m} = A_t p_c \frac{\gamma\sqrt{\left[\frac{2}{\gamma+1}\right]^{\frac{\gamma+1}{\gamma-1}}}}{\sqrt{\gamma R T_c}} \tag{4}$$

$$c^* = \frac{g_c P_c A_t}{\dot{m}} \tag{5}$$

$$\mathrm{Thrust} = \frac{c^* C_f\, \dot{m}}{g_c} \tag{6}$$

$$\mathrm{Isp} = \frac{c^* C_f}{g_c} \tag{7}$$

In addition, SCORES provides two flags to indicate the status of the flow through the nozzle. These flags indicate choked flow at the throat and the presence of a normal shock in the nozzle.

Uncertainty:

The solution procedure described thus far relies on several assumptions. These assumptions include infinitely fast chemical reactions in the combustor (equilibrium flow), perfect mixing of reactants, mixtures of perfect gasses, adiabatic flow, and infinitely slow reactions (frozen flow) throughout the nozzle. These assumptions result in idealized predictions, which do not account for real losses, and that may differ from the real processes by 10% or more.

A statistical approach to analyzing these errors provides not only improved estimation, but also a quantifiable uncertainty in the computational results of thrust and Isp. Writing the actual thrust and Isp as the product of their respective calculated values and a multiplier gives the following expressions:

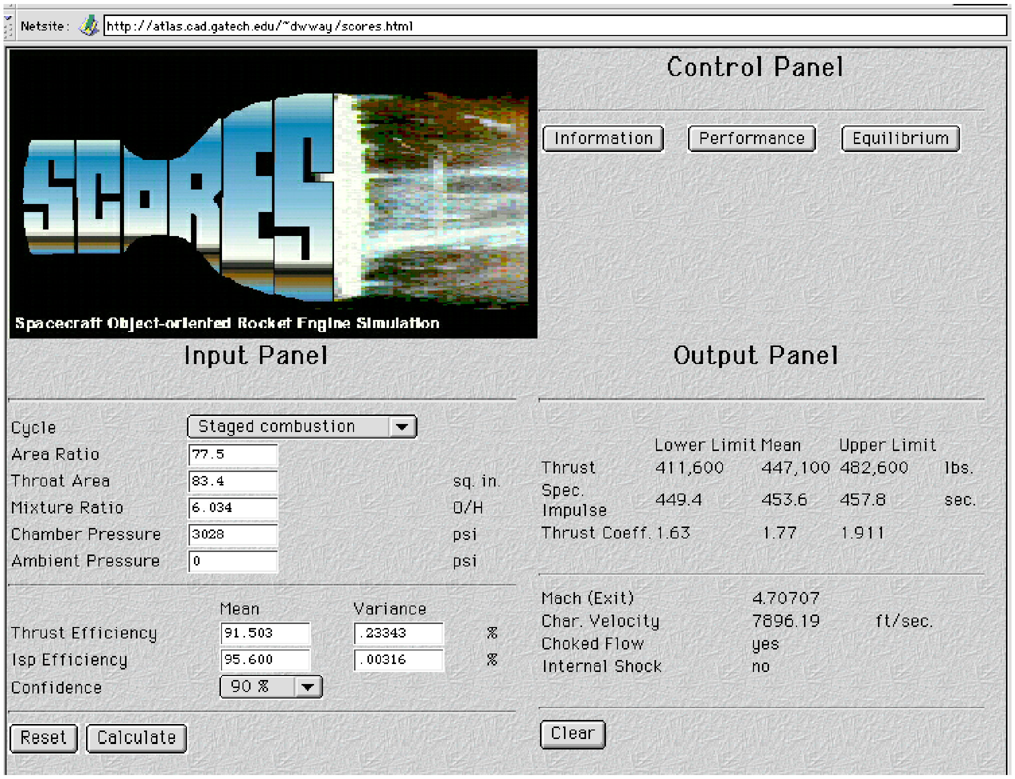
$$\begin{aligned} \beta_{thr} \times \text{Thrust}_{calc} &= \text{Thrust}_{act} \\ \beta_{Isp} \times \text{Isp}_{calc} &= \text{Isp}_{act} \end{aligned} \tag{8}$$

If the multipliers, β_{thr} and β_{Isp}, are normal distributions with known means and variances, then Thrust_{act} and Isp_{act} will also be normal distributions with predictable means and variances. Statistically, multiplying a normal distribution by a scalar results in a mean that is multiplied by that scalar and a variance that is multiplied by the square of the scalar. Working with distributions, rather than single values, allow the reporting of confidence intervals for both thrust and Isp in addition to their respective mean values. A 90% confidence interval will contain the true mean 90% of the time.

A calibration procedure determines the multipliers by comparing nominal results with known values for a sample of existing engines and then determining the statistical sample mean and variance. The reader is cautioned that determining the multipliers in this fashion limits their applicability to engines similar to the sample engines used in the calibration. Larger sample sizes, of course, lead to improved results.

Web Interface:

SCORES is equipped with a web interface. CGI scripts, written in Perl, accept input from HTML forms. This input is inserted into the appropriate input files and then piped through the executable application. The output generated by the executable is then parsed for the desired information, which is displayed in HTML format on a new web page.



http://atlas.cad.gatech.edu/~dwway/scores.html

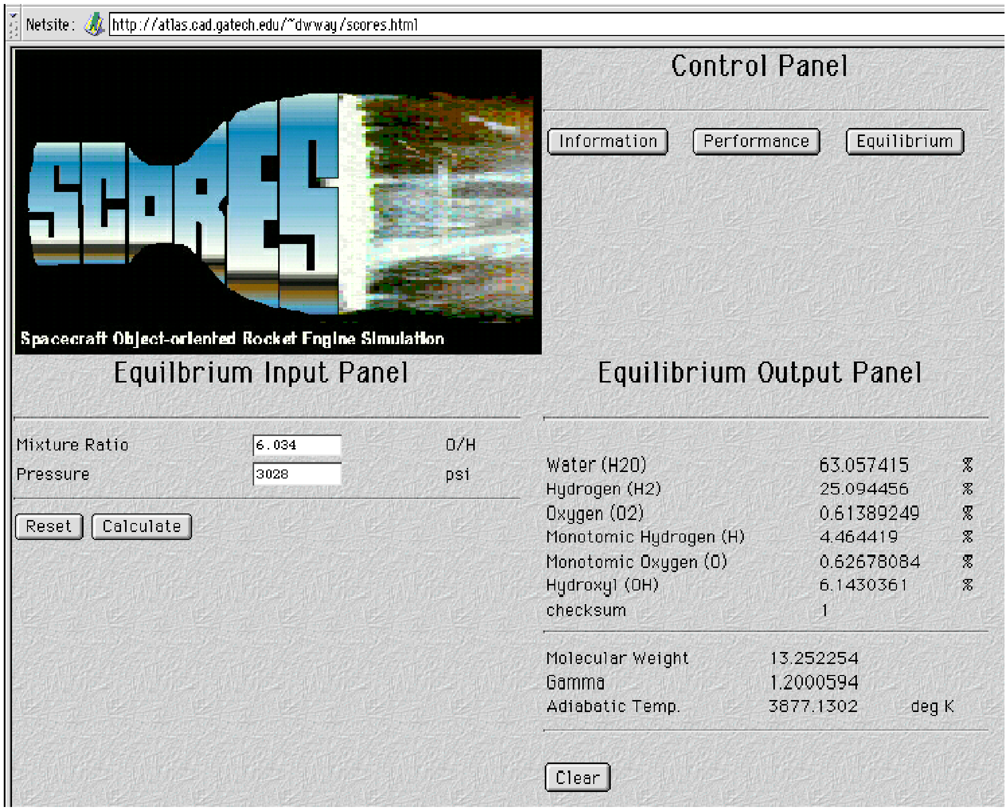
Cycle	Staged combustion	
Area Ratio	77.5	
Throat Area	83.4	sq. in.
Mixture Ratio	6.034	O/H
Chamber Pressure	3028	psi
Ambient Pressure	0	psi

	Mean	Variance	
Thrust Efficiency	91.503	.23343	%
Isp Efficiency	95.600	.00316	%
Confidence	90 %		

	Lower Limit	Mean	Upper Limit	
Thrust	411,600	447,100	482,600	lbs.
Spec. Impulse	449.4	453.6	457.8	sec.
Thrust Coeff.	1.63	1.77	1.911	

Mach (Exit)	4.70707	
Char. Velocity	7896.19	ft/sec.
Choked Flow	yes	
Internal Shock	no	

Figure 1 SCORES Performance



Mixture Ratio	6.034	O/H
Pressure	3028	psi

Water (H2O)	63.057415	%
Hydrogen (H2)	25.094456	%
Oxygen (O2)	0.61389249	%
Monotomic Hydrogen (H)	4.464419	%
Monotomic Oxygen (O)	0.62678084	%
Hydroxyl (OH)	6.1430361	%
checksum	1	

Molecular Weight	13.252254	
Gamma	1.2000594	
Adiabatic Temp.	3877.1302	deg K

Figure 2 SCORES Equilibrium

The current SCORES interface uses frames to organize the individual web pages. Buttons are available to access either the engine performance or equilibrium calculation portions of the system. The SCORES web site is public and can be accessed from the World Wide Web at the URL address listed below: http://atlas.cad.gatech.edu/~dwway/scores.html.

Providing a web interface for the program has several advantages. First, distribution is greatly simplified and portability is not a concern. It does not need to be re-compiled on another machine that may have a different C++ compiler. Also, version control is automatic. With a continually evolving program, as new versions are created they are automatically updated for all users. Finally, Providing a web based interface literally opens-up the system to be used by anyone. Anyone with a web browser may access the code. No programming is required and the intuitive nature of the input and output allow immediate use. In this manner, the web interface allows for multi-platform, graphically distributed users. Figure 2 shows a screen capture of the web interface provided for SCORES chemical equilibrium calculations.

RESULTS

The following section presents the results of a comparison used to validate SCORES solutions against accepted chemical equilibrium codes and historical data. This section first compares equilibrium predictions with those of accepted equilibrium codes STANJAN[2] and CEA[5] (Chemical Equilibrium Analysis). Second, performance predictions, thrust and Isp, are compared with actual engine data from the Chemical Propulsion Information Agency (CPIA)[6].

Equilibrium Comparisons:

First, a comparison was made to validate the equilibrium calculations. A full factorial array of five mixture ratios (O/F: 4.0 to 8.0) and five chamber pressures (P_c: 1000 to 3000 psia) produced 25 cases for comparison of equilibrium results. SCORES, STANJAN, and CEA were used to analyze each of the 25 cases. Mole fractions, temperature, and γ were recorded. In each case, the initial temperature of the reactants was 300 K.

Table 2 Mole Fraction Comparison

	H2O	H2	O2	H	O	OH
SCORES	0.6369	0.2512	0.0058	0.0452	0.0058	0.0551
CEA	0.6401	0.2508	0.0054	0.0440	0.0055	0.0542
STANJAN	0.6360	0.2517	0.0058	0.0447	0.0058	0.0560

Table 2 lists the mole fractions predicted by each code for one case (O/F=6.0 and Pc=1000 psia). This case was chosen to be representative of all the results. Similar results were found in all of the cases. Figure 3 shows graphically the similarity in the predictions of mole fractions for the major product species, H_2O and H_2.

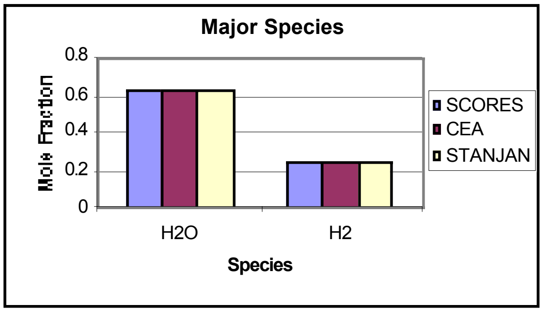


Figure 3 Major Species Mole Fraction

All three codes agreed to within 0.5% of mole fraction in all cases. SCORES agreed exceptionally well with STANJAN, predicting similar mole fractions within 0.15% in all cases. This close agreement with STANJAN is not surprising when considering that both programs utilize the same method of element potentials.

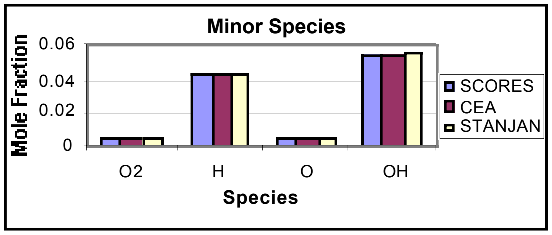


Figure 4 Minor Species Mole Fraction

Figure 4 above shows the correlation in the minor species: O2, H, O, and OH. Table 3 below records the results for temperature and γ for the representative case (O/F=6.0 and Pc=1000 psia).

Table 3 Temperature and Gamma

	T	gamma
SCORES	3604.52	1.2018
CEA	3594.49	1.1382
STANJAN	3601.54	1.1387

Figure 5 shows the comparison of adiabatic flame temperature. This plot shows Temperature as a function of mixture ratio for P_c= 1000 psia. The trends were similar for all other pressures. As with the mole fractions, temperature agreed exceptionally well, within 0.5% in all cases.

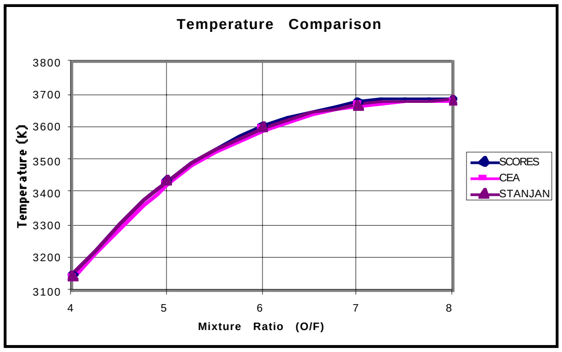


Figure 5 Adiabatic Flame Temperature

Figure 6 shows the ratio of specific heat comparison. This plot shows γ as a function of mixture ratio for P_c= 1000 psia. The trends were similar for all other pressures.

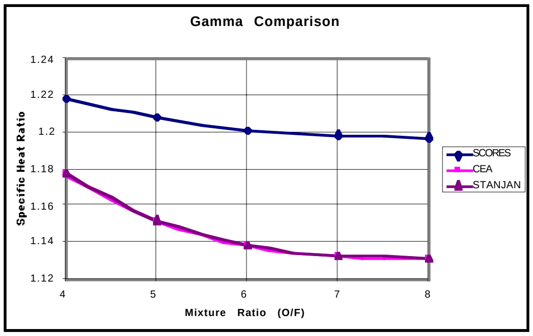


Figure 6 Ratio of Specific Heats

Figure 6 reveals a consistent over-prediction by SCORES. This error ranges from 3.5% to 5.5%. The error is believed to be due to the method in which SCORES predicts γ from the equation of state. Efforts are currently underway to improve the method for determining γ by first determining the speed of sound in the equilibrium gas mixture.

Engine Comparisons:

SCORES performance predictions were also compared to historical data from nine existing engines. In each case, SCORES was run at vacuum conditions using the engine data provided. The results for thrust and specific impulse were then compared with the advertised values for engine vacuum thrust and Isp. The ratio of the actual values to the predicted values determined the multipliers, β. These multipliers were compared and a sample mean and variance were calculated.

Table 4 Engine Data

Engine	ε	A_t (in^2)	O/F	P_c (psia)
J-2 (200K)	27.5	169.6	5	670
M-1	40	803.24	5	1100
RL10A-3-3	57	20.75	5	400
J-2 (225K)	27.5	169.8	5.5	670
J-2 (230K)	27.5	169.6	5.5	691
J-2S	40	116.9	5.5	1246
SSME	77.5	83.16	6.011	3277
RL10A-3-3A	61	19.2	5	475
RL10A-4	84	19.3	5.5	568

The CPIA/M5 Liquid Propellant Engine Manual[6] provided the engine data listed in Table 4 above. Nine Lox/Lh2 rocket engines were selected for comparison: 200K J-2, M-1, RL10A-3-3, 225K J-2, 230K J-2, J-2S, SSME, RL10A-3-3A, and RL10A-4.

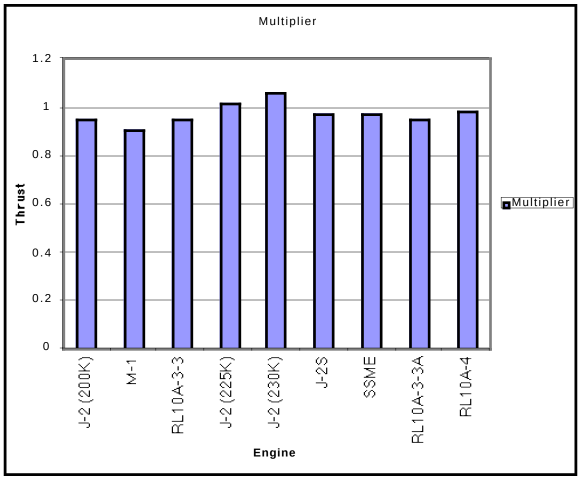


Figure 7 Thrust Comparison

Figure 7 shows the uncorrected thrust comparison. Table 5 below records the actual and predicted thrust values. . Actual values were taken from CPIA/M5. Predicted values are taken from SCORES at vacuum conditions with a multiplier of 100%.

Table 5 Thrust Comparison (lb.)

Engine	Actual	Predicted
J-2 (200K)	200,000	209,100
M-1	1,500,000	1,656,000
RL10A-3-3	15,000	15,740
J-2 (225K)	225,000	221,900
J-2 (230K)	230,000	216,000
J-2S	265,000	273,500
SSME	512,845	527,400
RL10A-3-3A	16,500	17,340
RL10A-4	20,800	21,130

The sample mean of the thrust multipliers was determined to be 0.9746. The maximum uncorrected error is 10.4%. Using the above mean value to calibrate the thrust calculations reduces this error to 8.5%. Figure 8 shows the comparison of Isp.

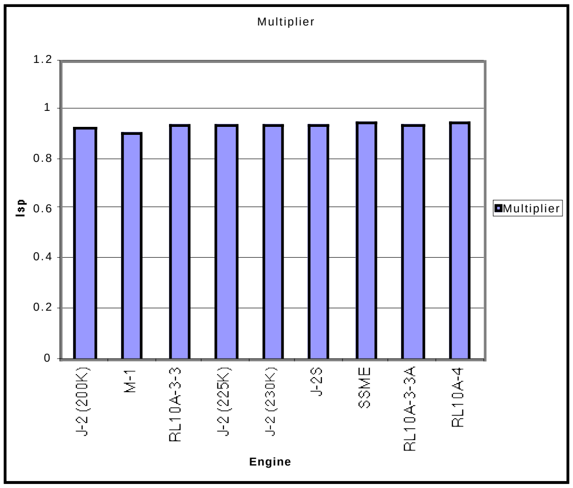


Figure 8 Isp Comparison

Table 6 below records the actual and predicted Isp values. Actual values were taken from CPIA/M5. Predicted values are taken from SCORES at vacuum conditions with a multiplier of 100%.

Table 6 Isp Comparison (sec)

Engine	Actual	Predicted
J-2 (200K)	426	461.8
M-1	428	473.1
RL10A-3-3	444	472.6
J-2 (225K)	422.6	452.6
J-2 (230K)	422.7	453
J-2S	435	465
SSME	452.9	475.5
RL10A-3-3A	444.4	475.1
RL10A-4	449	472.3

The sample mean of the Isp multipliers was determined to be 0.9342. The maximum uncorrected error is 10.5%. Using the above mean value to calibrate the Isp calculations reduces this error to 3.3%.

CONCLUSIONS

1. SCORES accurately predicts equilibrium mole fractions and adiabatic flame temperature over a wide range of operating conditions. SCORES agreed within 0.5% with both STANJAN and CEA. Mole fraction and temperature are important parameters in accurately predicting exhaust gas behavior. The thermodynamic behavior is, in turn, very important in modeling the effects of changes in engine parameters which affect combustion (mixture ratio and chamber pressure).

2. SCORES does not accurately predict specific heat ratio. 3.5% to 5.5% error in γ is unacceptable. Adiabatic flow relations are very sensitive to this parameter. Additional work is needed to improve this prediction. This work will center around methods to calculate the speed of sound in an equilibrium mixture of gasses. Engine performance calculations are expected to improve with improved γ predictions.

3. Errors in SCORES engine performance (thrust and Isp) calculations are within acceptable tolerances for use in conceptual-level design. Uncorrected, the thrust and Isp were found to be within 10% of the published values for nine rocket engines. More importantly for conceptual design and optimization, performance trends are properly predicted. Statistically correcting the calculations improved the errors to within 8.5% for thrust and 3.3% for Isp.

4. Statistical calibration of the performance predictions reduces the errors associated with real vs. idealized processes by 2 to 7%. This method additionally provides the engineer with additional information about the uncertainty of the calculations. This uncertainty information is provided in the form of confidence intervals.

5. Providing SCORES on the World Wide Web has been very effective. The web interface provided with SCORES represents an efficient method for users to interact with and use the software. As SCORES improves, changes are immediately incorporated.

FUTURE WORK

SCORES is an on-going effort to provide a useable analysis tool for the conceptual designer. The following list identifies areas for future work:

1. Add capability for sizing the nozzle throat to a desired thrust level. This is easily implemented with an additional iteration following performance calculations.
2. Include different propellant combinations, particularly LOX/RP-1. This requires the replacement of the current 2-D search with a constrained optimizer.
3. Improve the estimation of the frozen flow ratio of specific heats. This requires prediction of the speed of sound in the mixture of gasses.
4. Provide WER (weight estimation relationships) for low fidelity prediction of engine weight. This requires regression analysis of a propulsion database.
5. Add plotting capabilities to web-based output. This requires a plotting package.
6. Add capability to predict nozzle length. This may require a response surface approximation to method of characteristics results.
7. Include a top-level feed system cycle analysis. This would require additional information to be provided by the user to identify the feed system in use.
8. Provide options for both SI and English units to be used for either input or output. Most easily implemented by input and output scripts in the web-based version.
9. Provide an on-line user’s guide for documentation and instruction.

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