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CEA-Based Performance and Off-Design Assessment of LOX/Biofuel Rocket Propellant Candidates

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Research Article

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Abstract

This paper screens six LOX-compatible liquid fuels using NASA CEA: RP-1, dimethyl ether, ethanol, methanol, acetic acid, and formic acid. All fuels were calculated under one condition set: chamber pressure 20 bar, nozzle expansion ratio 40, fuel temperature 298 K, oxidizer temperature 90 K, and O/F sweep from 0.5 to 8.0. I kept these settings fixed because the aim was not to optimize an engine, but to compare the fuels under the same ideal thermochemical assumption before any CFD or experimental work. RP-1 gave the highest sampled vacuum specific impulse, 336.24 s at O/F = 2.5. DME came very close, reaching 334.61 s at O/F = 1.5. The difference was only 1.63 s in ideal vacuum specific impulse. At first, chamber temperature seemed to be the main reason for the ranking, but the results showed that molecular weight and characteristic velocity also controlled the final performance. DME did not match the RP-1 chamber temperature, but its lower product molecular weight helped it stay close. Ethanol reached 327.31 s, lower than DME, but its mean off-design degradation was slightly smaller. This makes ethanol a reasonable candidate where mixture-ratio tolerance is valued more than peak ideal performance alone. The result should be used only as an early CEA screening. Injector losses, finite-rate chemistry, cooling, density impulse, ignition behavior, feed-system mass, and mission-level constraints were not included.

Introduction

RP-1 was kept as the reference fuel in this study because it is still the practical benchmark for LOX/hydrocarbon rocket engines. It gives high energy release, good density, established handling practice, and a long engineering record. The other fuels were not selected to replace RP-1 directly. They were selected because oxygenated fuels such as DME, ethanol, and methanol are often considered for cleaner, smaller, or demonstrator-type propulsion systems [1–3]. Acetic acid and formic acid were added as lower-performance oxygenated cases so that the comparison did not include only the stronger candidates.

A common CEA setup was used because comparing fuels from different pressure, temperature, or nozzle assumptions can give a false ranking. The chamber pressure was fixed at 20 bar because the target was common-condition fuel screening, not chamber-pressure optimization. The expansion ratio was fixed at 40 to keep the nozzle effect the same for all cases. Fuel temperature was set at 298 K and LOX temperature at 90 K so that the reactant states remained simple and repeatable. These choices make the result easier to trace from the CEA input files.

The O/F ratio was swept from 0.5 to 8.0 for every fuel. This wide range was used because the oxygenated fuels were expected to peak at lower O/F values than RP-1. The internal oxygen inside DME, ethanol, methanol, and the acid fuels reduces the amount of external oxidizer required. In the results, RP-1 peaked at O/F = 2.5, while DME, ethanol, and methanol peaked at O/F = 1.5. This shift was expected, but the lower optimum O/F did not automatically mean higher specific impulse.

The main comparison was based on vacuum specific impulse. I also calculated an off-design degradation index because a fuel with a high peak value may still lose performance quickly when O/F changes. That behavior matters in early engine studies, especially for small engines where mixture ratio may not remain exactly at the best point during operation. RP-1 stayed strongest in both peak performance and O/F tolerance. DME was closest to RP-1 in peak ideal performance. Ethanol was lower in peak value, but its mean degradation was slightly better than DME.

This work is not a final propellant-selection study. It does not include injector pressure loss, atomization, evaporation, finite-rate reaction, wall heat loss, cooling design, density impulse, tank size, ignition, toxicity, or material compatibility. The purpose is narrower: to identify how these fuels behave under one ideal equilibrium CEA framework and to decide which candidates deserve higher-fidelity CFD, experiment, or system-level analysis next.

Literature Review

RP-1 has remained the main reference fuel for LOX hydrocarbon engines because its performance, density, handling, and engine heritage are well established. Edwards reviewed the long development of liquid hydrocarbon fuels and showed why kerosene-type fuels became practical for aerospace propulsion rather than only thermochemically strong candidates [1]. Sutton and Biblarz also treat LOX/RP-1 as a standard benchmark for comparing hydrocarbon rocket performance [4]. For this reason, RP-1 was not used here as a renewable fuel option, but as the reference line that the other fuels had to approach.

Earlier LOX/hydrocarbon studies also show that fuel comparison cannot be judged from heat release alone. Orton et al. studied LOX/hydrocarbon auxiliary propulsion options and showed that engine-level selection depends on more than ideal combustion temperature [2]. In CEA-type calculations, final vacuum specific impulse depends on chamber temperature, characteristic velocity, thrust coefficient, specific heat ratio, and exhaust molecular weight. This point became clear in the present calculation also. DME did not have the highest chamber temperature, but it remained close to RP-1 because its product molecular weight was lower.

Green-propellant screening work by Burkhardt et al. is directly related to this paper because it compared several LOX/fuel combinations using theoretical CEA-type data [3]. Their dataset included LOX/RP-1, LOX/DME, LOX/ethanol, and LOX/methanol. The same general ranking appeared in the present work: RP-1 remained highest, DME came close, ethanol followed, and methanol stayed below ethanol. The present values were lower by about 4.3–5.0%, mainly because the chamber pressure and input assumptions were not identical. I used that comparison only for trend checking, not as experimental validation.

Ethanol has a separate history in small and non-toxic rocket propulsion. NASA-related OMS/RCS studies considered LOX/ethanol as a safer alternative for some propulsion applications [7,14]. Mota et al. also modeled a LOX/ethanol liquid rocket engine and showed that ethanol remains relevant for small engine analysis and educational propulsion work [8]. In the present CEA sweep, ethanol did not beat DME in

peak vacuum specific impulse. Its peak value was 327.31 s, while DME reached 334.61 s. But ethanol had slightly lower mean off-design degradation than DME, so it should not be rejected only from peak I_{sp}.

Most previous studies report peak performance or engine design behavior, but fewer compare peak value and mixture-ratio tolerance together under one simple screening framework. This is the gap addressed here. The paper does not claim final propellant selection. It only compares six LOX/fuel cases using one CEA setup and then adds an off-design degradation index to see how quickly each fuel loses performance when O/F moves away from its best sampled point.

Computational Method

CEA case setup

NASA CEA was used in equilibrium rocket mode to compare six LOX/fuel cases: RP-1, DME, ethanol, methanol, acetic acid, and formic acid. All fuels were calculated at the same chamber pressure of 20 bar, expansion ratio of 40, fuel temperature of 298 K, and LOX temperature of 90 K. These settings were kept fixed because the aim was fuel screening, not engine optimization. The O/F ratio was swept from 0.5 to 8.0 for every fuel. This range was selected to capture both fuel-rich and oxidizer-rich behavior under one common setup. It was also needed because oxygenated fuels were expected to peak at lower O/F values than RP-1.

From each CEA run, chamber temperature, vacuum specific impulse, characteristic velocity, thrust coefficient, specific heat ratio, and molecular weight were extracted. No correction was added for injector loss, heat loss, finite-rate chemistry, cooling, or feed-system effects. The reported values are therefore ideal CEA screening results, not direct engine-test predictions.

Optimum point and off-design metric

The optimum point of each fuel was taken as the sampled O/F value that produced the highest Isp,vac. A finer O/F grid could shift the exact optimum slightly, so the values reported here are best-sampled values rather than interpolated maxima. This approach was chosen to keep the comparison tied directly to the CEA output table. To compare off-design behavior, the following degradation index was calculated at each sampled O/F point:

$$\Delta I_{sp} = (I_{sp,vac,opt} - I_{sp,vac}) / I_{sp,vac,opt} \quad (1)$$

A low value of Delta_Isp means that the fuel keeps more of its own best performance at that O/F point. The mean, 95th-percentile, and maximum values of this index were used to summarize the loss across the sweep. The final interpretation was not based on a weighted score. Peak $I_{sp,vac}$ was treated as the main performance measure, and the degradation statistics were used to judge mixture-ratio tolerance.

Results and Discussion

Vacuum specific impulse

Figure 1 shows the vacuum specific impulse trends for the six fuels. RP-1 gives the highest sampled value, 336.24 s at O/F = 2.5. DME is very close, with 334.61 s at O/F = 1.5. Ethanol and methanol form the next group, reaching 327.31 s and 322.09 s, respectively. Acetic acid and formic acid fall well below the other fuels, with maximum values of 290.76 s and 237.53 s.

The result is useful because the ranking does not follow chamber temperature alone. DME does not reach the highest temperature, but it remains close to RP-1 because its equilibrium products are relatively light. Ethanol shows the same trend, although with a larger penalty in c* and peak Isp. The two acid fuels show the opposite behavior: their oxygen-rich structure leads to lower heat release and heavier exhaust products in this calculation set.

Chamber temperature and molecular weight

The chamber-temperature curves in Fig. 2 and the optimum-point map in Fig. 3 explain the performance order more clearly. RP-1 reaches 3477.44 K at its optimum. DME and ethanol are lower at 3322.90 K and 3253.65 K. Methanol is slightly cooler than ethanol, and the acid fuels are much cooler, especially formic acid.

Molecular weight changes the interpretation. DME gives the lightest equilibrium products among the leading candidates, with MW = 21.706 at its best sampled point. Ethanol is also light, at MW = 21.963, while RP-1 is slightly heavier at MW = 22.764. This is why DME remains close to RP-1 even without matching the RP-1 chamber temperature. Methanol has a heavier product mixture, and the acid fuels are penalized by both lower temperature and higher MW.

Characteristic velocity and thrust coefficient

Figure 4 shows that RP-1 and DME form the leading pair in characteristic velocity. Their optimum *c** values are 1775.6 m/s and 1777.8 m/s. Ethanol follows at 1747.6 m/s, while methanol drops to 1684.7 m/s. The acid fuels are substantially lower.

The thrust coefficient values in Table 1 are close enough that they do not change the main ranking. Methanol and acetic acid have comparatively high Cf values, but their lower c* and less favorable molecular weights dominate the final Isp,vac. This is why a single-parameter explanation would be misleading for these fuels.

Table 1
Best sampled CEA values for each fuel in the O/F sweep.

Fuel	O/F_{opt}	$I_{sp,vac}$ (s)	T_c (K)	c^* (m/s)	C_f	$\varvec{\gamma}$	MW
RP-1	2.5	336.24	3477.44	1775.6	1.8570	1.1324	22.764
DME	1.5	334.61	3322.90	1777.8	1.8457	1.1309	21.706
Ethanol	1.5	327.31	3253.65	1747.6	1.8367	1.1324	21.963
Methanol	1.5	322.09	3225.45	1684.7	1.8749	1.1192	23.657
Acetic acid	1.0	290.76	3075.10	1520.5	1.8754	1.1165	27.732
Formic acid	0.5	237.53	2472.94	1280.6	1.8190	1.1414	30.820

The optimum O/F location also shifts with fuel type. RP-1 peaks at O/F = 2.5, whereas DME, ethanol, and methanol peak at O/F = 1.5. The optimum shifts even lower for the two acids. This is consistent with the internal oxygen in the fuel molecules, but the lower oxidizer requirement does not automatically produce higher specific impulse.

Off-design mixture-ratio behavior

Table 2 and Figs. 5–7 summarize how much performance is lost away from the best sampled O/F point. RP-1 is still the strongest overall case, with the lowest mean degradation, 95th-percentile degradation, and maximum degradation. Among the renewable-type candidates, ethanol and DME are close. Ethanol has a slightly smaller mean degradation, while DME has a slightly smaller maximum degradation.

This is the main reason ethanol should not be dismissed only because its peak Isp is lower than DME. DME is the better candidate when the objective is to approach RP-1 peak performance. Ethanol is more balanced when some tolerance to mixture-ratio variation is also valued. Methanol is weaker because it trails ethanol in both peak performance and off-design behavior. The acid fuels are the least attractive in both measures.

Table 2
Off-design performance degradation calculated relative to each fuel's own best sampled $I_{sp,vac}$.

Fuel	Mean ΔI_{sp}	95th-percentile ΔI_{sp}	Maximum ΔI_{sp}
RP-1	0.129	0.265	0.335
Ethanol	0.173	0.312	0.325
DME	0.175	0.314	0.328
Methanol	0.216	0.381	0.394
Acetic acid	0.269	0.441	0.453
Formic acid	0.388	0.560	0.570

Table 3
Benchmarking Against Published CEA-Type Data

Fuel	Peak performance	O/F tolerance	Engineering interpretation
RP-1	1st	1st	Reference case; highest Isp,vac and best robustness in the sweep.
DME	2nd	3rd	Closest renewable-type candidate to RP-1 in peak ideal performance.
Ethanol	3rd	2nd	Lower peak than DME, but slightly better mean off-design behavior.
Methanol	4th	4th	Lower *c** and heavier products keep it below ethanol.
Acetic acid	5th	5th	Not competitive for the selected LOX equilibrium case.
Formic acid	6th	6th	Lowest performance; high penalty in temperature and MW.

Benchmarking Against Published CEA-Type Data

The present values were compared with the open ODE/CEA86 dataset reported by Burkhardt et al. [3]. That source is useful because it includes LOX/RP-1, LOX/ethanol, LOX/methanol, and LOX/DME in one theoretical dataset. The pressure in that study was 1.034214 MPa and the expansion ratio was 40. The present work uses 20 bar and its own reactant-state assumptions, so the comparison is not a strict validation. It is used only to check whether the relative trend is reasonable.

Table 4
Trend-level comparison with the open ODE/CEA86 dataset of Burkhardt et al. [3]. Deviation = 100 x (present - reported) / reported.

Fuel	Reported $I_{sp,Vac}$ (s)	Present $I_{sp,Vac}$ (s)	Deviation (%)	Condition difference	Assessment
RP-1	353.9 @ R = 2.62	336.24	-4.99	Pressure and input-state assumptions differ.	Same highest-performance trend.
Ethanol	342.4 @ R = 1.81	327.31	-4.41	Pressure and reactant-state assumptions differ.	Trend agrees; ethanol remains below DME and RP-1.
Methanol	336.4 @ R = 1.39	322.09	-4.25	Different code setup and state assumptions.	Trend agrees; methanol remains below ethanol.
DME	350.2 @ R = 1.72	334.61	-4.45	Pressure differs; open DME/LOX comparisons are limited.	Trend agrees; DME remains close to RP-1.

The present values are lower than the benchmark values by about 4.3-5.0%. Because the operating conditions and input handling are not identical, this level of difference is acceptable for trend comparison. More importantly, the relative order is preserved: RP-1 is highest, DME is the strongest oxygenated challenger, ethanol follows, and methanol remains below ethanol. This agreement supports the use of the present dataset for preliminary screening, but it should not be described as experimental validation.

Practical Implications and Limitations

For a launch vehicle or high-performance engine study, the present result still favors RP-1. DME is the closest non-RP-1 case in ideal CEA performance and deserves attention in future screening. Ethanol is also important because it combines acceptable ideal performance with relatively good O/F tolerance and a long history in small rocket-engine development. For laboratory or educational demonstrators, ethanol may therefore be easier to justify than its peak Isp alone suggests.

The limitations are important. The analysis does not include finite-rate chemistry, injector pressure loss, atomization, vaporization, ignition transients, combustion instability, heat transfer to the wall, regenerative cooling, density impulse, tank and feed-system mass, toxicity, material compatibility, or mission-level optimization. The results should not be used by themselves to select a flight propellant. They are best used as a first screening step before higher-fidelity engine and system analysis.

The current dataset is also not large enough for a formal uncertainty-quantification study. A future study should vary chamber pressure, expansion ratio, fuel temperature, oxidizer temperature, and O/F ratio together. Only then would polynomial-chaos or Sobol-type sensitivity analysis be meaningful [9–12]. In

this paper, the uncertainty-related discussion is therefore limited to a proposed future workflow, not a reported result.

Reproducibility Note

To make the calculation traceable, each fuel was treated as a separate CEA case using the same chamber pressure, expansion ratio, and reactant temperatures. The raw output table was then reduced to the quantities reported in Tables 1 and 2. The degradation metric was calculated directly from the sampled $I_{sp,vac}$ values without curve fitting. A finer O/F interval is recommended in future work if the exact optimum mixture ratio is required.

Conclusions

This study compared six LOX/fuel combinations in NASA CEA under one common setup: 20 bar chamber pressure, expansion ratio 40, fuel temperature 298 K, LOX temperature 90 K, and O/F sweep from 0.5 to 8.0. The fixed setup was used to screen fuel chemistry before moving to CFD, hot-fire testing, or system-level design. RP-1 remained the benchmark. It gave the highest sampled vacuum specific impulse, 336.24 s at O/F = 2.5, and also showed the lowest off-design degradation across the O/F range. This confirms why RP-1 is still difficult to replace when ideal performance and mixture-ratio tolerance are considered together. DME was the closest fuel to RP-1 in peak CEA performance. It reached 334.61 s at O/F = 1.5, only 1.63 s lower than RP-1. DME did not reach the RP-1 chamber temperature, but its lower equilibrium molecular weight and high characteristic velocity helped it stay close. For peak ideal performance, DME was the strongest oxygenated candidate in this calculation.

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Figures

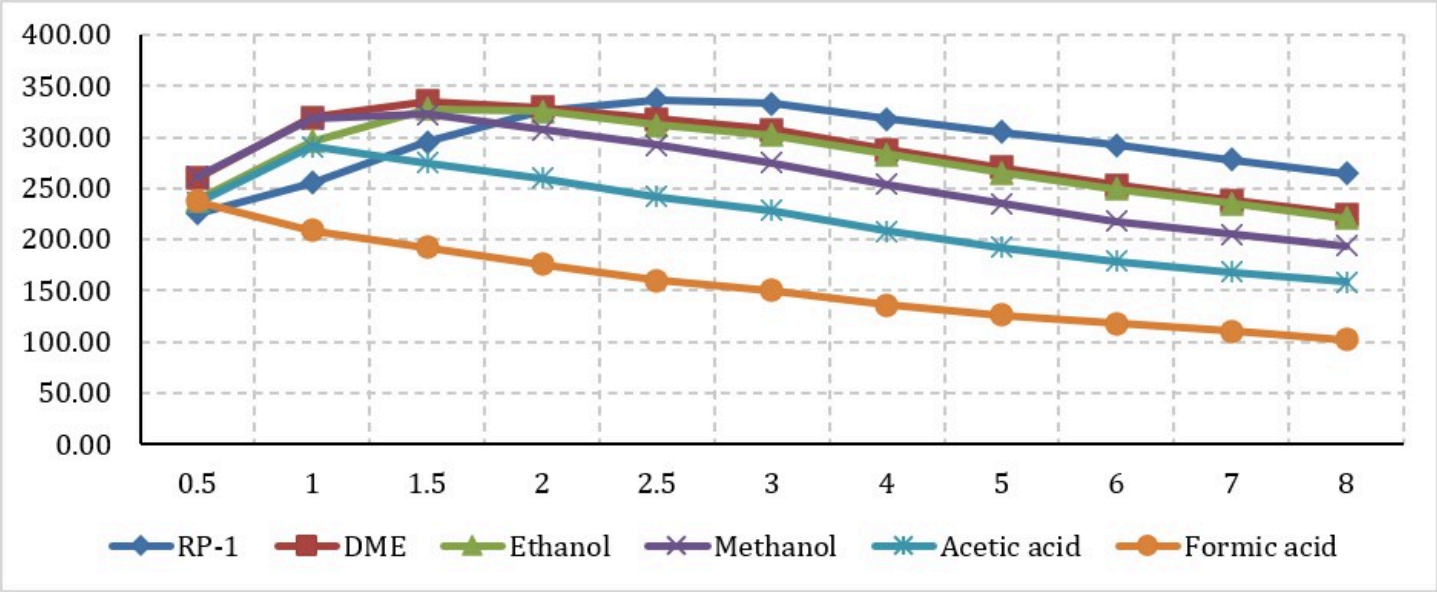


Figure 1

Vacuum specific impulse vs O/F ratio for the selected 20 bar, expansion-ratio-40 LOX cases.

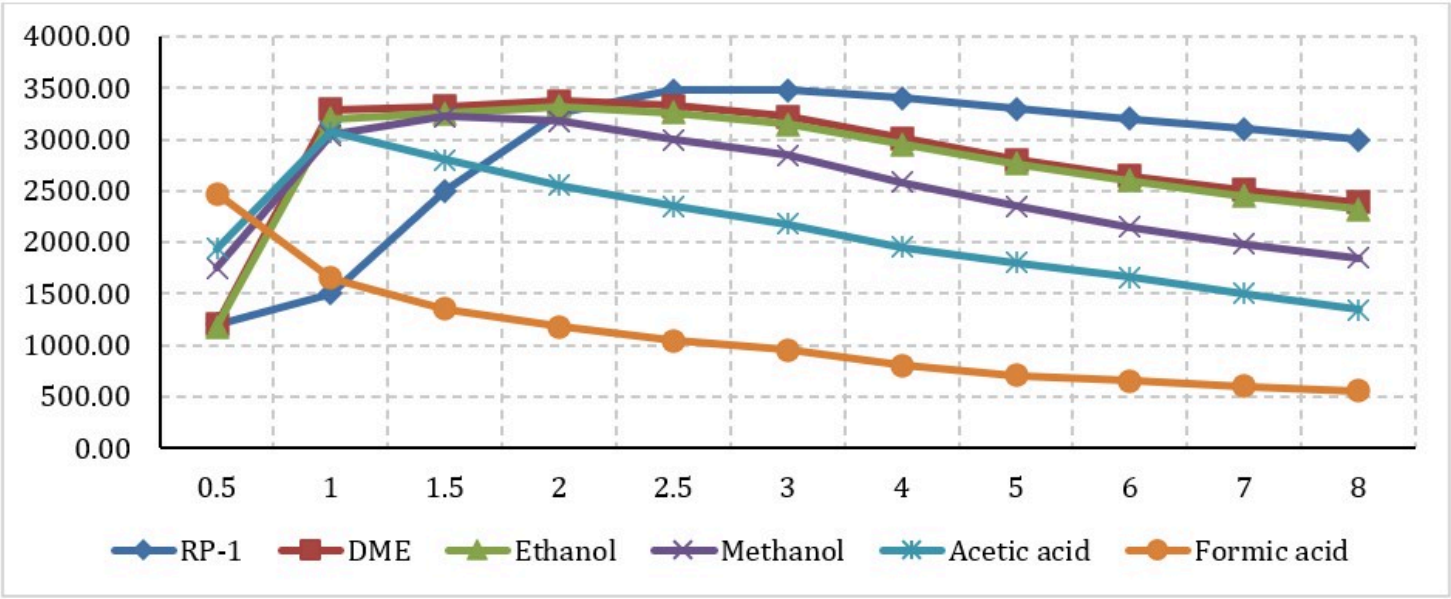


Figure 2

Chamber temperature vs O/F ratio ratio for the six LOX/fuel combinations.

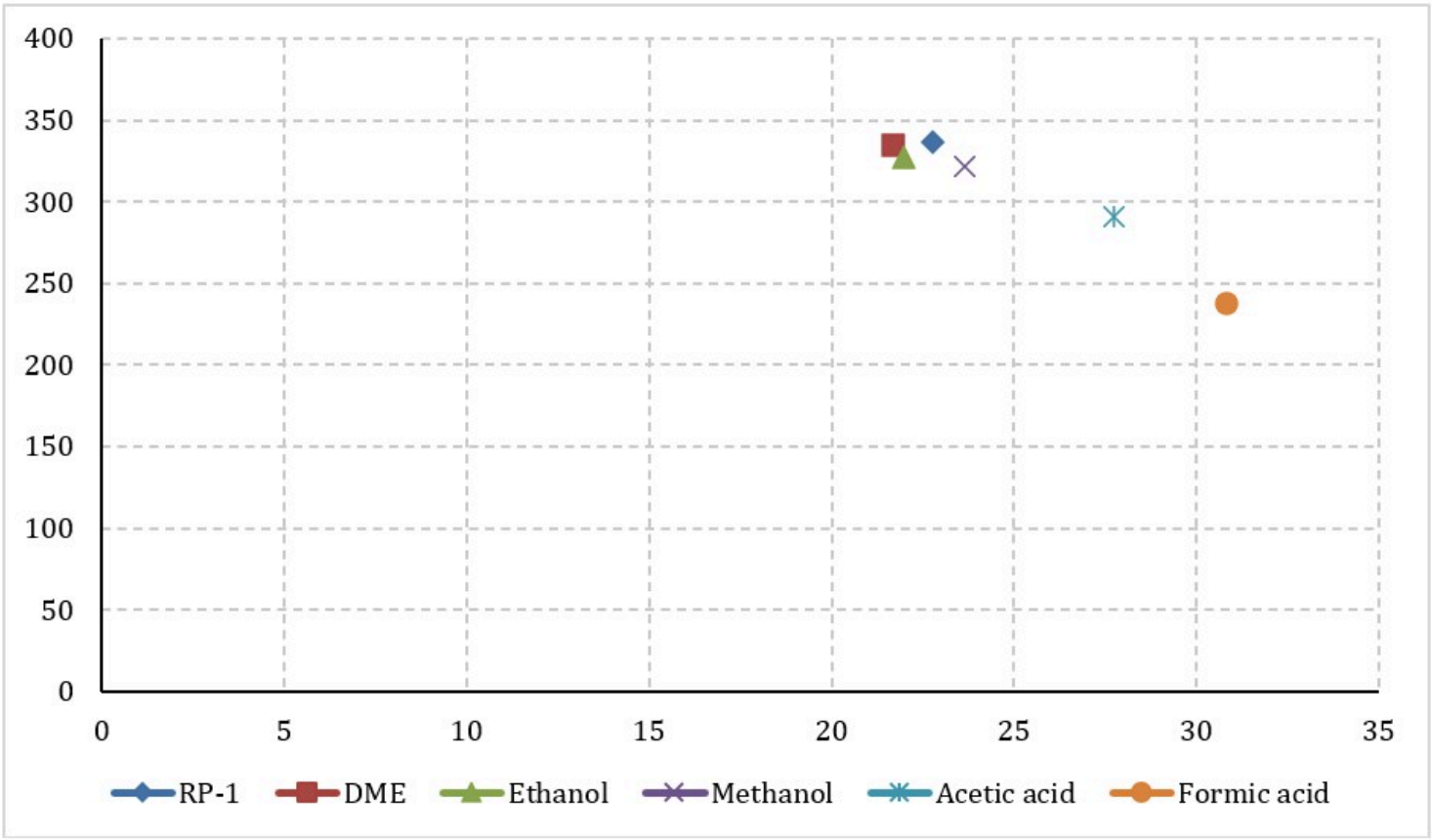


Figure 3

Optimum I_{sp} versus molecular weight, point size represents chamber temperature.

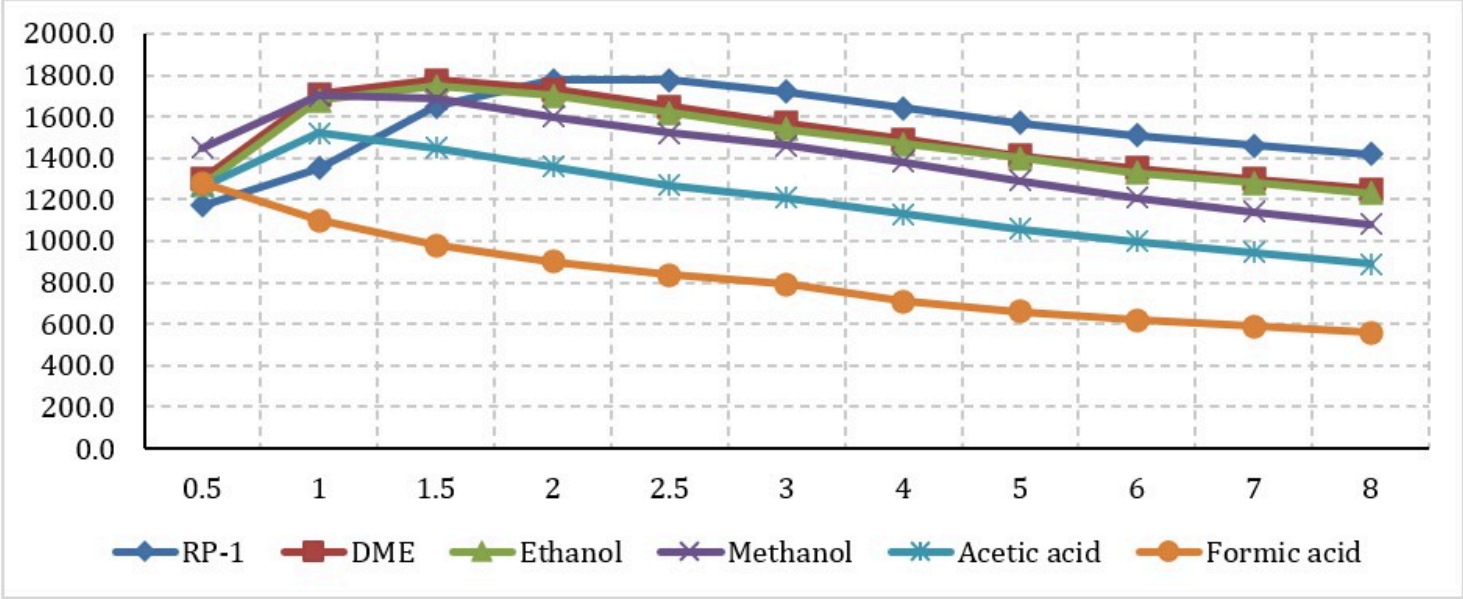


Figure 4

Characteristic velocity vs O/F ratio obtained from the CEA sweep.

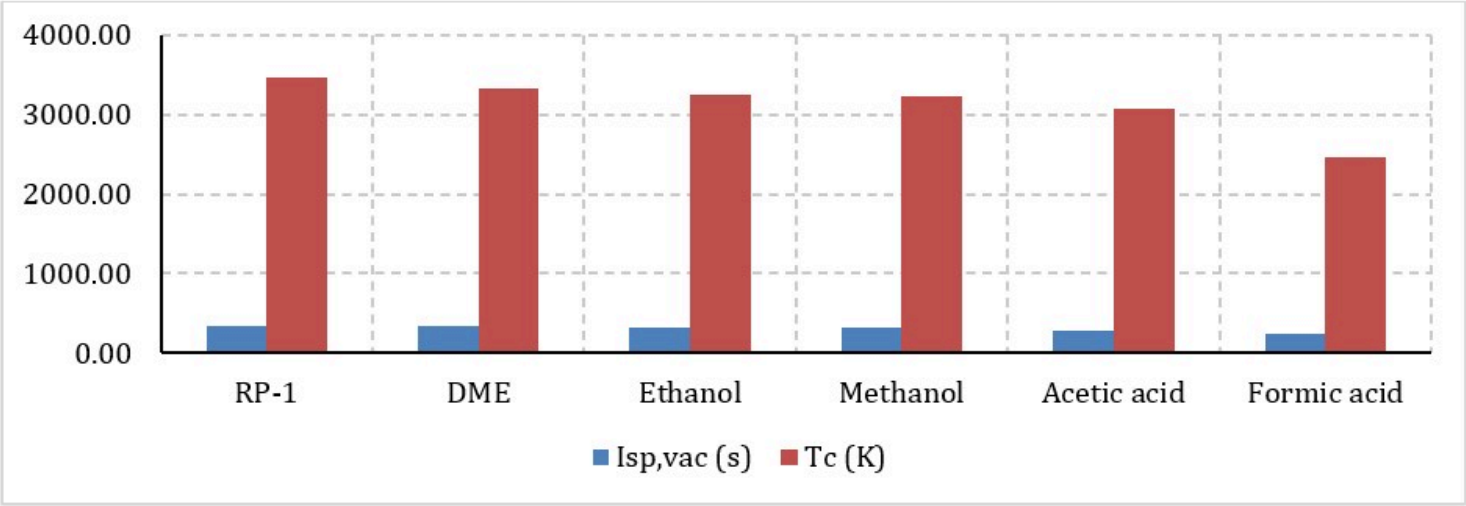


Figure 5

Optimum-point comparison of vacuum specific impulse and chamber temperature.

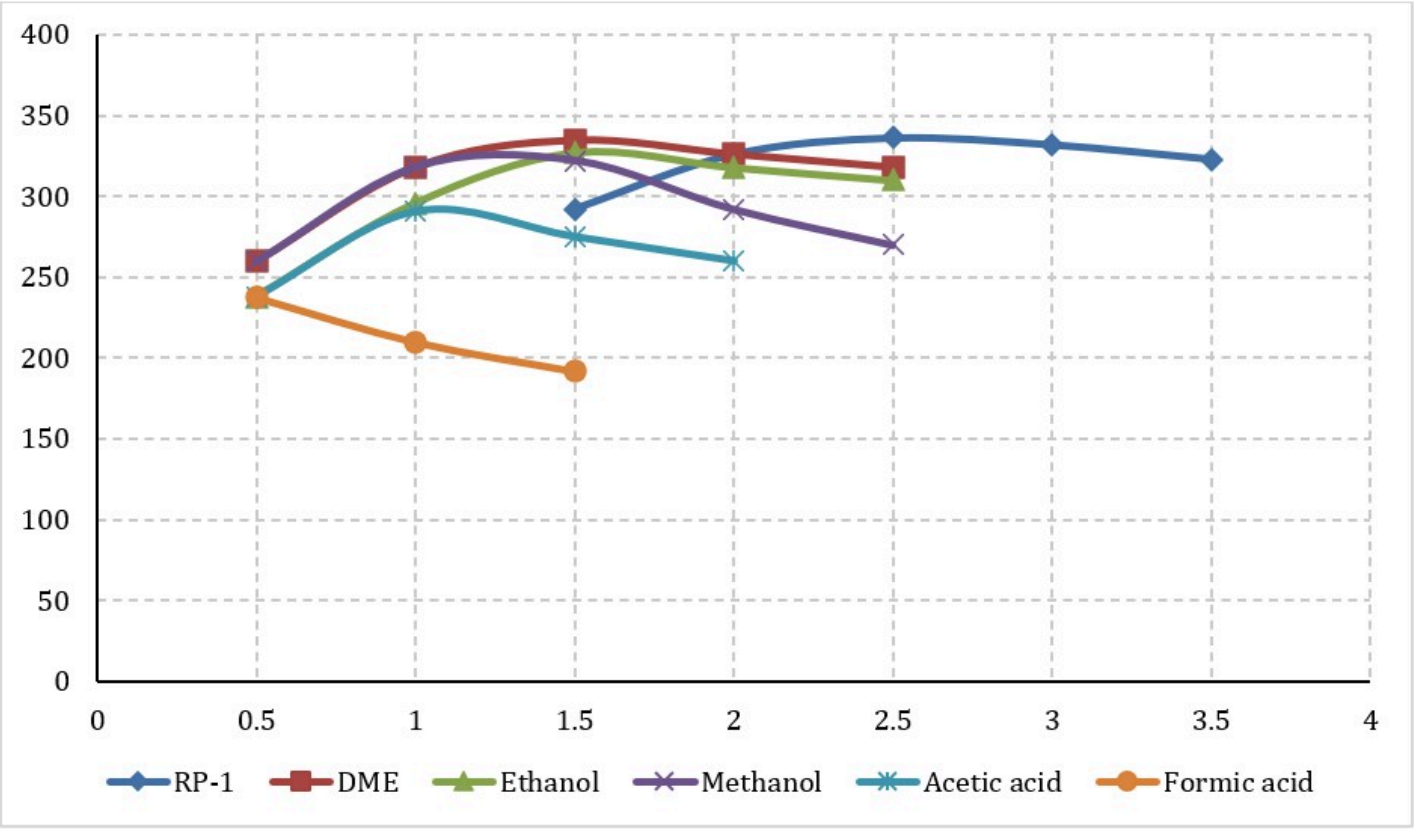


Figure 6

Near-optimum I_{sp} response around the sampled maximum for each fuel.

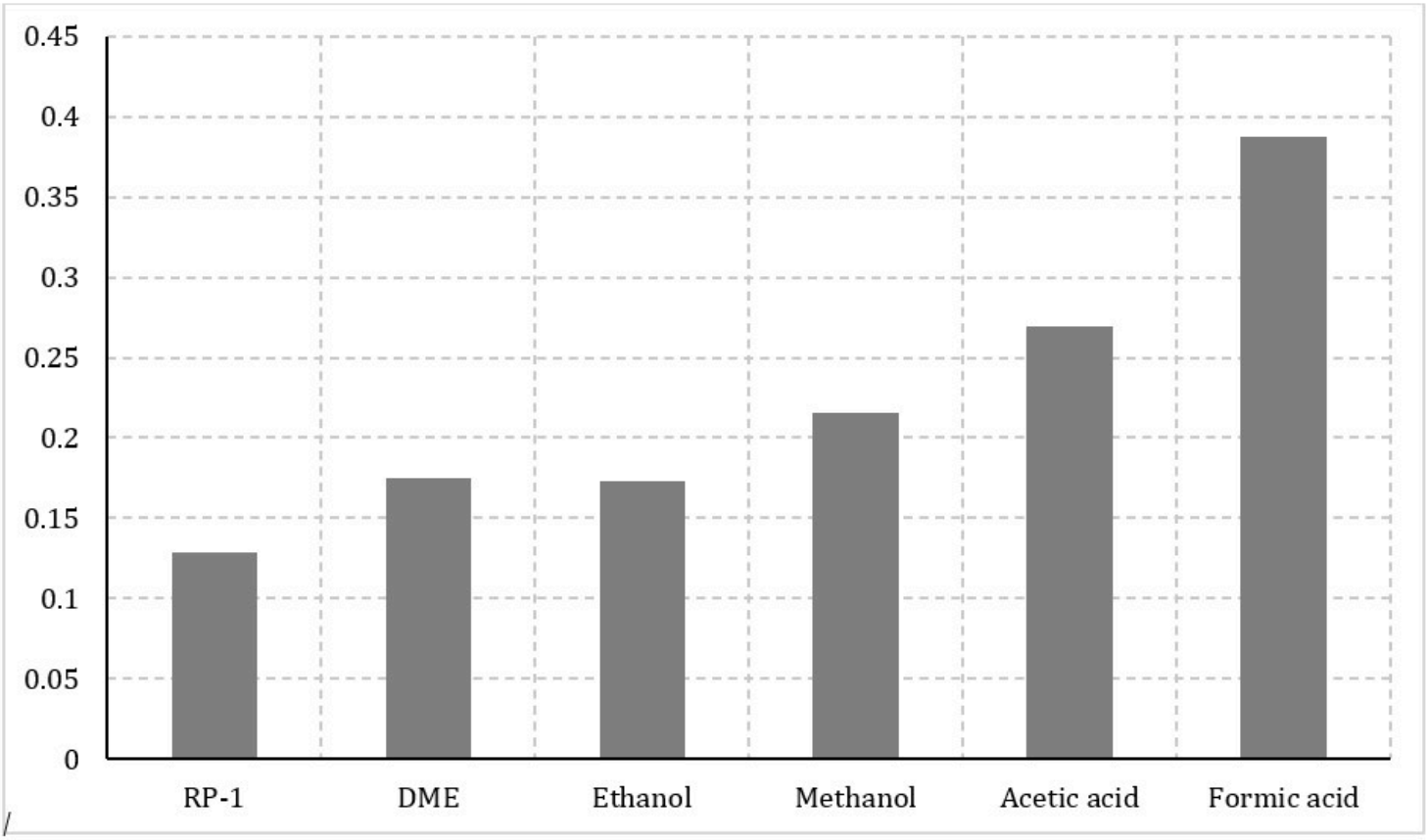


Figure 7

Mean off-design degradation of $^{\Delta}I_{sp}$ across the O/F sweep.