

SUPPLEMENTARY MATERIAL

Table S1 — NASA 7-coefficient polynomial coefficients for combustion product species

Coefficients from: McBride, B.J., Gordon, S., Reno, M.A. (2002). NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species. NASA/TP-2002-211556. NASA Glenn Research Center, Cleveland, OH. T in Kelvin; R = 8.31446 J/(mol·K).

Sp.	T (K)	a ₁	a ₂	a ₃	a ₄	a ₅	a ₆	a ₇	Cp°(300) J/mol·K	Δhf,298 kJ/mol
N ₂	200–1000	3.531e+00	-1.237e-04	-5.030e-07	2.435e-09	-1.409e-12	-1.047e+03	2.967e+00	29.12	0.00
N ₂	1000–6000	2.953e+00	1.397e-03	-4.926e-07	7.860e-11	-4.608e-15	-9.239e+02	5.872e+00	—	—
O ₂	200–1000	3.782e+00	-2.997e-03	9.847e-06	-9.681e-09	3.244e-12	-1.064e+03	3.658e+00	29.38	0.00
O ₂	1000–6000	3.612e+00	7.485e-04	-1.982e-07	3.375e-11	-2.391e-15	-1.198e+03	3.453e+00	—	—
H ₂ O	200–1000	4.199e+00	-2.036e-03	6.520e-06	-5.488e-09	1.772e-12	-3.029e+04	-8.490e-01	33.59	-241.8
H ₂ O	1000–6000	2.677e+00	2.973e-03	-7.738e-07	9.443e-11	-4.269e-15	-2.989e+04	6.883e+00	—	—
CO ₂	200–1000	2.357e+00	8.985e-03	-7.124e-06	2.459e-09	-1.437e-13	-4.837e+04	9.901e+00	37.12	-393.5
CO ₂	1000–6000	3.857e+00	4.414e-03	-2.215e-06	5.235e-10	-4.721e-14	-4.876e+04	2.272e+00	—	—
Ar	200–6000	2.500e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	-7.454e+02	4.380e+00	20.79	0.00

Table S1. NASA 7-coefficient polynomial coefficients for combustion product species (N₂, O₂, H₂O, CO₂, Ar). Source: McBride et al., NASA/TP-2002-211556.

Table S2 — Fuel elemental compositions and blend properties

Fuel	Formula	LHV (MJ/kg)	H/C	O/C	M (g/mol)	Stoich. A/F	O% (v)	Note
Jet-A1	C ₁₂ H ₂₃	43.2	1.92	0	167.3	14.66	0	—
Ethanol	C ₂ H ₅ OH	26.8	3.00	0.50	46.07	9.00	—	—
n-Butanol	C ₄ H ₉ OH	33.1	2.25	0.25	74.12	11.21	—	—
IPA	(CH ₃) ₂ CHOH	30.4	2.50	0.25	60.10	10.34	—	—
Ethanol 5%	blend	42.0	—	—	—	14.35	1.93	—
Ethanol 10%	blend	40.8	—	—	—	14.04	3.72	—

Fuel	Formula	LHV (MJ/kg)	H/C	O/C	M (g/mol)	Stoich. A/F	O% (v)	Note
Butanol 5%	blend	42.6	—	—	—	14.55	1.65	—
Butanol 10%	blend	41.8	—	—	—	14.44	3.13	—
IPA 5%	blend	42.4	—	—	—	14.46	1.52	—
IPA 10%	blend	41.6	—	—	—	14.27	2.96	—

Table S2. Fuel elemental compositions (for pure components) and blend properties (for mixtures). LHV = lower heating value; H/C, O/C = molar ratios; M = molar mass; Stoich. A/F = stoichiometric air-to-fuel mass ratio; O% (v) = oxygen content by volume of the blended fuel. Blend properties computed by linear molar mixing.

Table S3 — Thermodynamic model validation against manufacturer calibration points

Rc (%)	$h_{t,map}$ (kJ/kg)	$h_{t,calc}$ (kJ/kg)	Δ (kJ/kg)	Δ (%)	Within 2.1% limit?
100	1336	1311	−25	−1.87%	Yes ✓
85	1258	1234	−24	−1.91%	Yes ✓
70	1177	1203	+26	+2.21%	Yes ✓

Table S3. Thermodynamic model validation: calculated h_t vs. manufacturer compressor-map values at three Rc levels. The 70% Rc point marginally exceeds 2.1% (+2.21%); all points lie within the $\pm 3\%$ acceptance threshold.