

Supplementary Material: Launch Emission Assessment Tool (LEAT v1.0): Part I - Development of a tool to calculate altitude-dependent rocket launch emissions for use in chemistry-climate models

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Abstract.

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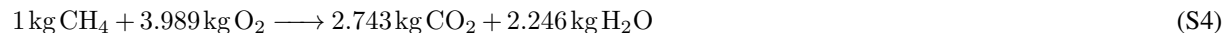
S1 Additional Tables

5 S1.1 Stoichiometric equation

LOX/LH2



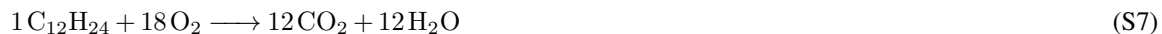
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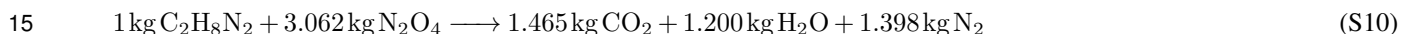
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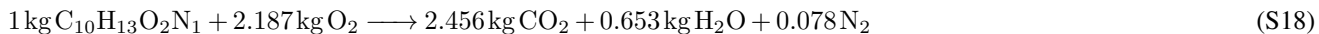
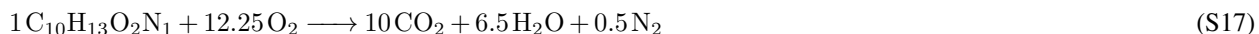
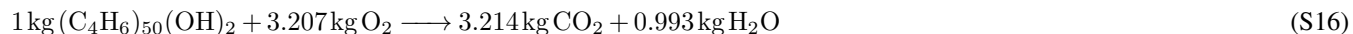
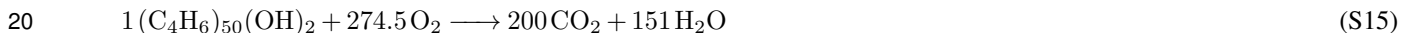
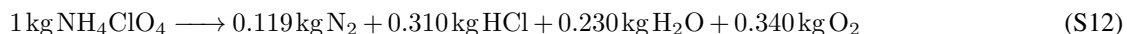
LOX/RP-1



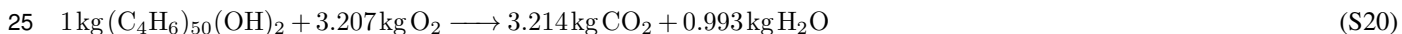
NTO/UDMH



Solid



LOX/HTPB



S1.2 Emission indices in literature

Table S1. LOX/LH2 emissions in kg/kg burned propellant

ROF	7.94:1 (stoic.)	6:1 (typ.)	4.9:1 (max ^a)	Ryan 2022	Larson 2017	Ross 2014	Ross ^c 2009	James ^d 2021	Pradon 2023	Brown 2024	Barker 2024
H ₂ O	1	1.277	1.515	1	-	1	1.24	0.965	1.27	1	1.058
H ₂	-	-	-	-	-	-	-	0.035	-	-	0.035
Sum	1	1.277	1.515	1	-	1	1.24	1	1.27	1	1.093
NOx	-	-	-	0.033	0.033	-	0.02	-	-	0.033	-

Table S2. LOX/CH4 emissions in kg/kg burned propellant

ROF	3.99:1 (stoic.)	3.6:1 (typ.)	3.5:1 (max ^a)	James 2021	Barker ^d 2024
CO ₂	0.550	0.596	0.610	0.360-0.492	0.426
CO				0.051-0.189	0.12
OH				0-0.002	
H ₂				0.002-0.011	0.006
H ₂ O	0.450	0.488	0.499	0.439-0.452	0.446
Sum	1	1.085	1.109	0.852-1.146	0.998
BC				0.005	0.998
NOx				-	0.005

Table S3. LOX/RP-1 emissions in kg/kg burned propellant

ROF	3.43:1 (stoic.)	2.36:1 (typ.)	2.8:1 (max ^a)	Ryan 2022	Larson 2017	Ross 2014	Ross ^c 2009	FAA 2020	James 2021	Pradon 2023	Brown 2024	Barker ^d 2024
CO	-	-	-	-	-	-	-	0.2476	0.240-0.399	-	-	0.318
CO ₂	0.710	0.934	0.826	-	-	0.6	0.88	0.4062	0.335-0.470	0.91	0.6	0.637
H ₂	-	-	-	-	-	-	-	-	0.006-0.015	-	-	0.01
H ₂ O	0.290	0.382	0.338	0.3	-	0.35	0.3	0.2434	0.250-0.284	0.36	0.35	0.34
Sum	1	1.316	1.164	0.3	-	0.95	1.18	0.897	0.581-0.884	1.27	0.95	1.305
BC	-	-	-	0.035	-	0.01-0.04	0.05 ^c	0.005	0.025	-	0.02	0.022
NOx	-	-	-	0.014	0.014±0.003	-	0.02	0.0121 ^b	-	-	0.014	-

Table S4. N₂O₄/UDMH emissions in kg/kg burned propellant

ROF	3.06:1 (stoic.)	2.1:1 (typ.)	2.9:1 (max ^a)	Ryan 2022	Ross 2014	Ross ^c 2009	James ^d 2021	Pradon 2023	Brown 2024	Barker ^d 2024
CO ₂	0.361	0.472	0.376	-	0.15	0.63	0.289	0.46	0.2	0.15
CO				-	-	-	0.069	-	-	0.069
H ₂				-	-	-	0.004	-	-	0.004
H ₂ O	0.295	0.387	0.307	0.55	0.55	0.25	0.29	0.38	0.55	0.392
N ₂	0.344	0.451	0.359	-	-	0.29	0.348	-	-	-
Sum	1	1.31	1.042	0.55	0.7	1.17	1	0.84	0.75	0.615
BC				0.004	0.02-0.08	0	0.025	-	0.02	0.016
NOx				0.02	-	0.02	-	-	0.02	0.01

Table S5. Solid emissions in kg/kg burned propellant

ROF	HTPB 69:19:12	PBAN 69:19:12	Ryan 2022	Ross 2014	Ross ^c 2009	Pradon 2023	Brown 2024	James ^d 2021	Barker ^d 2024
CO ₂	0.386	0.295	-	0.2	0.27	0.44	0.3	0.013-0.048	0.112
CO	-	-	-	-	-	-	-	0.188-0.251	0.227
OH	-	-	-	-	-	-	-	0-0.006	-
H ₂ O	0.278	0.237	0.34	0.35	0.48	0.39	0.37	0.055-0.13	0.302
N ₂	0.082	0.091	-	-	0.08	-	-	0.081-0.094	-
HCl	0.214	0.214	0.21	-	0.15	0.22	-	0.194-0.212	-
Cl	-	-	0.003	-	-	-	0.21	0.003-0.022	0.217
Al ₂ O ₃	0.359	0.359	0.38	0.01-0.12	0.33	0.34	0.38	0.3-0.359	0.328
Sum	1.319	1.196	0.933	0.56 - 0.67	1.31	1.39	1.26	0.834 - 1.122	1.186
BC	-	-	0.004	0.02-0.08	-	-	0.02	0.025	0.016
NOx	-	-	0.003	-	0.02	-	0.003	0-0.001	-

Table S6. Hybrid (N₂O₄/HTPB) emissions in kg/kg burned propellant

ROF	4.61:1 (stoic.)	5.2:1 (typ.)	3.1:1 (max)	Ryan 2022	Ross 2014	James ^d 2021
CO ₂	0.573	0.518	0.784	-	0.2	0.24
CO						0.099
H ₂						0.001
H ₂ O	0.177	0.160	0.242	0.3	0.2	0.1
N ₂	0.250	0.226	0.342	-	-	0.558
Sum	1.000	0.905	1.369	0.300	0.400	0.998
BC	-	-	-	0.035	0.02-0.08	0.025
NOx	-	0.706 ^c	-	0.014	-	0.004

a) maximum ISP_{vac} calculated assuming $p_c=100$ bar, $A_e/A_t=50$ and equilibrium burning

b) after mixture with atmosphere

c) Ross 2009 does not distinguish between CO₂ and CO as well as H₂O and H₂, or ClOx and HOx and NOx

30 d) Primary emissions (mentioned here as secondary vary with altitude)

e) N₂O₄ is emitted expected to react to NO₂

For hydrazine engines, Ryan et al. (2022) only considered water vapour emissions. NOx emissions were assumed according to Larson et al. (2017) based on International Civil Aviation Organization database emissions and adapted to H₂-engines. For LOX/RP-1, in addition to the sources mentioned so far, there is also the Falcon 9 environmental report with detailed lists of emissions Federal Aviation Administration (2020). These are not based on an equilibrium calculation. Values from James et al. (2021) and Barker et al. (2024) represent primary emissions at engine level. These publications consider afterburning and are therefore not directly used for the emission calculation.

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S1.3 Measurement data from literature

Table S7. Measurement data from literature

Author	Year	Launch Vehicle	Time	Altitude	Species	Measurement value	Unit
Ross et al. (1997)	1997	Titan IV	29-30 min	18.9 km	CL2	126±44	ppbv
Newman et al.	2001	Soyuz	9-12 days	20 km	CN	up to 1000	cm ³
					N2O	210-230	ppbv
Popp et al. (2002)	2002	Athena 2	3.7-36.2 min	16-18.6 km	NO2	2.7±0.6	g/kg
					CO2	382	g/kg
					H2O	300	g/kg
Danilin et al. (2003)	2003	Athena 2	3.7-36.2 min	16-18.6 km	Al2O3	362	g/kg
					HCl	217	g/kg
					NO	2-4	g/kg
SABRE Barker et al. (2026)	2023	Falcon 9	41-45 min	15.72 - 15.87 km	NOx	17.0±2.7 / 7.1±0.6	ppb

S1.4 Alumina particle formation

The implementation of particle sizes are currently not in the tool but mentioned here for discussion. Solid propellants produce solid aluminium particles in addition to black carbon particles. Their formation is described in more detail in the literature. Hermsen Hermsen (1981) give a particle distribution as a function of the nozzle throat diameter based on measured values. The corresponding formula is

$$d_{Al} = 3.6304(25.4d_t)^{0.2932}(1 - \exp(-0.0008163\varepsilon_c P_c 6894,76\tau)) \quad (\text{S21})$$

with d_{Al} the mass-weighted average diameter in μm , d_t the throat diameter in mm, ε_c the concentration of Al_2O_3 in the chamber in g-mole/100 g, P_c the chamber pressure in Pa and τ the average chamber residence time in ms. Agglomeration also occurs here, so that the particles occur in different size distributions. Simmons et al. Simmons (2000) speak of an initial distribution of $2 \mu\text{m}$ and a secondary distribution by agglomeration of $100 \mu\text{m}$.

S1.5 Trajectory parameters

This is a detailed list of selected parameters from the *scenario_input.xlsx*:

Table S8. Selected scenario parameters for emission calculation

scenario	2025_Starship_IFT8	2023-013_Starlink5492	2025_Ariane_VA263
launch_vehicle	Starship V2.0 RTLS	Falcon-9 v1.2 (Block5) ADSL	Ariane 62
date	2025-03-06T23:30:31	2023-01-26T09:32:20	2025-03-06T16:24:00
launch_site	SB-OLPA	CC-LC40	CSG-ELA4
inclination	26.4	43.00	98
azimuth	94.82	56.37	351.96
mass_payload	8000	16800	3700
h_gt_start	50	140	60
h_gt_end	100	190	110
gamma_gt_total	0.5	1.5	1.6
t_startup	4	4	0
t_fr_start	48	53	50
t_fr_end	75	65	70
force_reduced	0.75	0.6	0.8

S1.6 Engine parameters

Table S9. Engine parameters for exhaust calculation

	Raptor	Vulcain 2.1	Vulcain 2.1 GG	Merlin 1D	Merlin 1D GG	P120C	
p_c	300	118.8	130	97	200	105	bar
a_e/a_t	34.34	32	2.3	16	1.36	11	-
ROF	3.6	6.03	0.9	2.36	0.3	69/19/12	-
fuel	CH ₄	LH2	LH2	RP-1	RP-1	APN/AL/HTPB	
oxidizer	O2	O2	O2	O2	O2		

For the Merlin 1D gas generator a ratio of the massflow $m_{GG}/m_{CC} = 0.0427$ was chosen based on Federal Aviation Administration (2020). For the Vulcain

50 2.1 gas generator a ratio of the massflow $m_{GG}/m_{CC} = 0.01534$ was chosen based on Safran.

S1.7 Total emission species

Table S10. Falcon 9 launch total min and max emissions up to 100 km in kg. Sum represents sum of species in table, not total emissions.

	Barker	LEAT CEA Equilibrium		LEAT CEA Frozen		LEAT Cantera	
	total	min	max	min	max	min	max
CO2	363904	109225	246721	105625	244830	125175	226083
CO	10801	56200	143710	57400	145999	55977	120449
H2O	143872	82503	114643	83964	115094	92186	107132
OH	0	12	2549	28	2831	112	8399
NO	1982	0	2526	0	2690	6	12770
NO2	0	0	4	0	4	0	11
O	0	0	301	0	352	1	2480
H	0	7	61	14	79	15	185
H2	0	2047	5721	1978	5550	1460	3693
BC	2658	2658	2658	2658	2658	2658	2658
Sum	523217	252652	518893	251667	520086	277590	483860

Table S11. Falcon 9 launch total emissions up to 100 km in kg for each x_{ab} . Sum represents sum of species in table, not total emissions.

x_{ab}	Barker	LEAT CEA Equilibrium				LEAT CEA Frozen				LEAT Cantera			
	N/A	1.2	2	4	8	1.2	2	4	8	1.2	2	4	8
CO2	363904	109248	142896	217243	246698	105635	140189	214393	244819	125187	156819	196949	226066
CO	10801	143696	122280	74962	56214	145992	124000	76773	57407	120342	100189	74596	55990
H2O	143872	82503	96810	108881	114643	83964	97688	109352	115094	92246	99904	103745	107060
OH	0	13	409	1953	896	31	542	2180	1032	112	2901	6959	7713
NO	1982	0	109	2081	1382	0	140	2221	1503	6	1017	6059	12770
NO2	0	0	0	1	4	0	0	1	4	0	0	3	11
O	0	0	18	209	112	0	26	244	133	1	387	1788	2340
H	0	9	29	35	34	17	43	48	46	17	99	129	128
H2	0	5721	4076	2628	2047	5550	3958	2550	1978	3690	2584	1880	1460
BC	2658	2658	2658	2658	2658	2658	2658	2658	2658	2658	2658	2658	2658
Sum	523217	343847	369286	410651	424688	343847	369244	410422	424674	344259	366557	394766	416195

Table S12. Starship launch total min and max emissions up to 100 km in kg. Sum represents sum of species in table, not total emissions.

	Barker total	LEAT CEA Equilibrium		LEAT CEA Frozen		LEAT Cantera	
		min	max	min	max	min	max
CO2	1741913	1334643	1549851	1302136	1509592	1337621	1491421
CO	58264	145990	282960	171647	303684	184060	282755
H2O	1490571	1348485	1394015	1340479	1380251	1355914	1385823
OH	0	6867	14135	15483	23837	1783	25037
NO	17134	56	4817	201	6598	75	9974
NO2	0	0	3	0	4	0	5
O	0	428	863	1444	2225	15	2251
H	0	338	383	632	702	62	289
H2	0	5847	11341	6519	11372	6568	10980
BC	4942	4942	4942	4942	4942	4942	4942
Sum	3312825	2847596	3263311	2843483	3243207	2891040	3213476

Table S14. Ariane 6 launch total min and max emissions up to 100 km in kg. Sum represents sum of species in table, not total emissions.

	Barker total	LEAT CEA Equilibrium		LEAT CEA Frozen	
		min	max	min	max
CO2	125631	13629	78987	13507	78888
CO	2308	16242	57839	16304	57916
H2O	243122	58489	98085	58303	98144
N2	0	23496	42522	21694	22939
HCl	38685	45443	56813	45600	56824
Cl	4896	1471	8734	1473	8718
Cl2	16268	1	7634	1	7496
Al2O3	90462	98959	99001	98957	98998
OH	0	84	2493	88	2511
NO	2110	10	2720	12	2702
NO2	0	0	3	0	3
O	0	4	446	4	443
H	0	90	216	93	220
H2	0	2221	6614	2228	6631
BC	2078	2078	2078	2078	2078
Sum	525561	262218	464185	260342	444512

Table S13. Starship launch total emissions up to 100 km in kg for each x_{ab} . Sum represents sum of species in table, not total emissions.

x_{ab}	Barker	LEAT CEA Equilibrium				LEAT CEA Frozen				LEAT Cantera			
		1.2	2	4	8	1.2	2	4	8	1.2	2	4	8
CO2	1741913	1334643	1372296	1461849	1549851	1302136	1338205	1418094	1509592	1337793	1371003	1435263	1490752
CO	58264	282960	258995	201999	145990	303684	280727	229881	171647	282245	260701	219786	184365
H2O	1490571	1348486	1358920	1377894	1394015	1340479	1348824	1363920	1380251	1359219	1367637	1378273	1382699
OH	0	6867	7824	11459	13741	15483	17224	21531	23286	1783	4770	13660	25037
NO	17134	56	210	1342	4817	201	660	2474	6598	75	366	2695	9974
NO2	0	0	0	0	3	0	0	1	4	0	0	1	5
O	0	428	456	631	849	1444	1545	1901	2198	15	111	742	2251
H	0	358	368	376	349	693	700	691	633	62	126	214	285
H2	0	11341	10106	7759	5847	11372	10327	8392	6519	10921	9679	7871	6616
BC	4942	4942	4942	4942	4942	4942	4942	4942	4942	4942	4942	4942	4942
Sum	3312825	2990080	3014118	3068253	3120405	2980434	3003154	3051828	3105669	2997055	3019336	3063448	3106926

Table S15. Ariane 6 launch total emissions up to 100 km in kg for each x_{ab} . Sum represents sum of species in table, not total emissions.

x_{ab}	Barker	LEAT CEA Equilibrium				LEAT CEA Frozen			
	N/A	1.2	2	4	8	1.2	2	4	8
CO2	125631	13629	52994	71155	78987	13507	52693	71043	78888
CO	2308	57839	32785	21227	16242	57916	32975	21297	16304
CH4	0	0	0	0	0	0	0	0	0
H2O	243122	71941	85507	88182	90143	71796	85679	88127	90064
N2	0	23496	25003	30893	42522	22930	22183	22397	22699
HCl	38685	56566	52696	53760	47071	56574	52727	53780	47230
Cl	4896	2392	6146	4705	4011	2385	6115	4699	3995
Cl2	16268	1	15	428	7634	1	14	415	7496
Al2O3	90462	98965	98980	98992	98998	98963	98977	98990	98996
OH	0	311	1565	997	887	344	1581	1022	913
NO	2110	101	1681	1188	548	123	1665	1192	551
NO2	0	0	1	3	2	0	1	3	2
O	0	10	189	170	196	11	189	170	196
H	0	154	150	139	131	158	154	143	135
H2	0	6614	3846	2832	2221	6631	3860	2840	2228
BC	2078	2078	2078	2078	2078	2078	2078	2078	2078
Sum	525561	334099	363637	376749	391672	333417	360892	368197	371775

S2 Additional Figures

S2.1 Trajectory subroutine

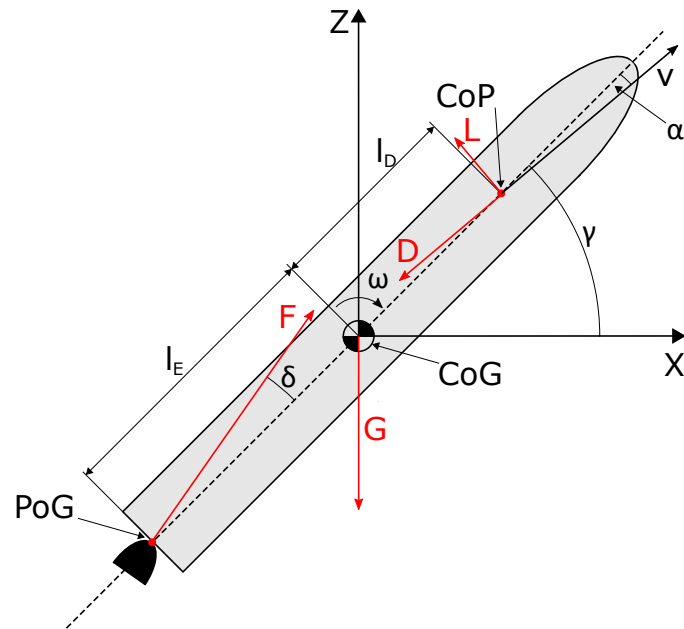


Figure S1. Forces and parameters for trajectory calculation during the ascend.

D = Drag [N]

F = Thrust [N]

G = Gravitation [N]

L = Lift [N]

l_D = Leverage arm drag force [m]

l_E = Leverage arm thrust force [m]

v = Flight path velocity [m/s]

m = Mass of total system [kg]

α = Angle of attack [°]

γ = Angle to ground [°]

δ = Angle of gimbal [°]

ω = Rotational speed around Y-axis [°/s]

CoG = Center of gravity

CoP = Center of pressure

PoG = Point of gimbal

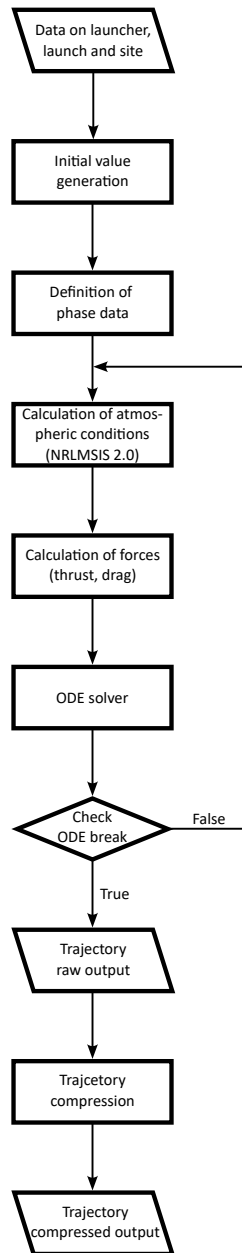


Figure S2. Schematic overview of the trajectory calculation logic. Rectangles represent programmes, trapezoids represent inputs/outputs, and diamonds represent decisions. The program calculates the ascent trajectory by solving the equations of motion and consideration of atmospheric conditions with the NRLMSIS model. Further details are explained in the main text.

S2.2 Emission calculation

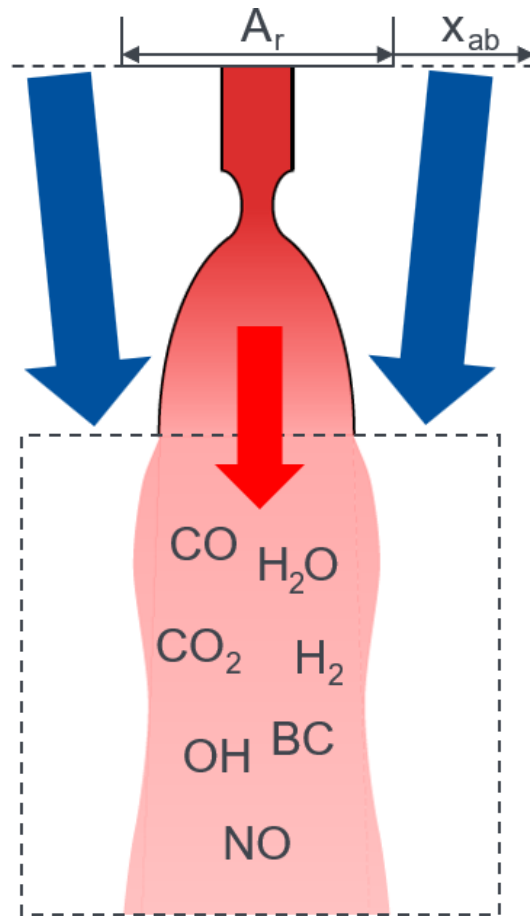


Figure S3. Afterburning control volume with incoming engine exhaust (red) and ambient air (blue). Incoming massflow of air is dependent on uncertainty factor x_{ab} which defines the A_{air} dependent on rocket area A_r

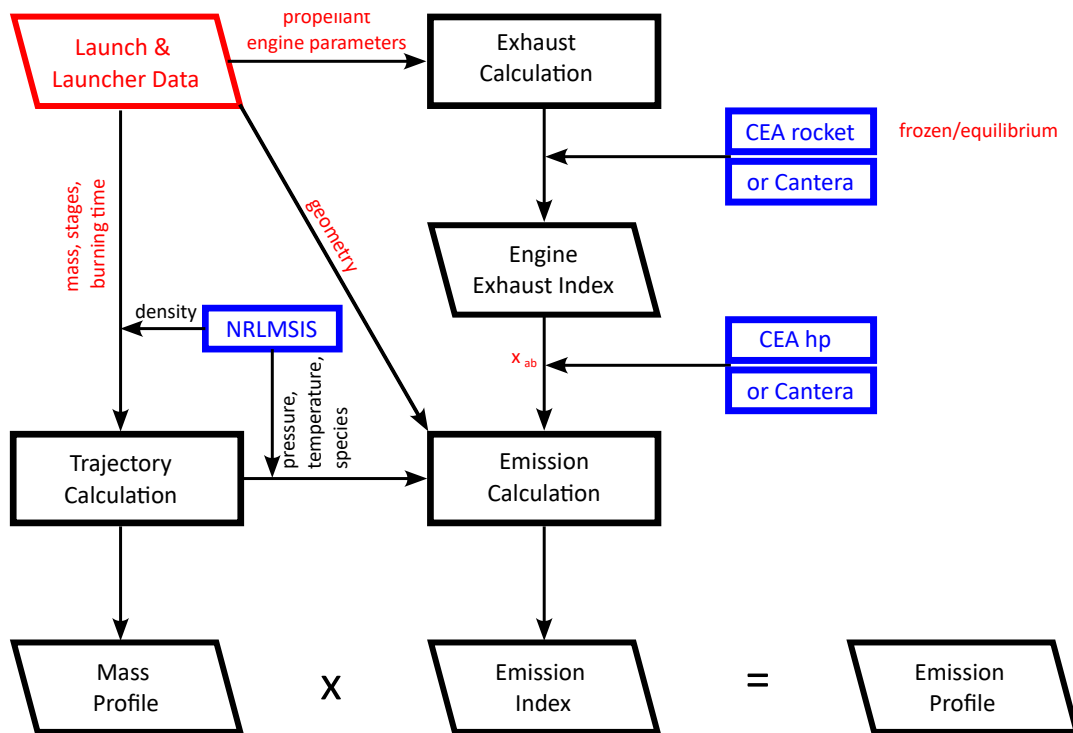
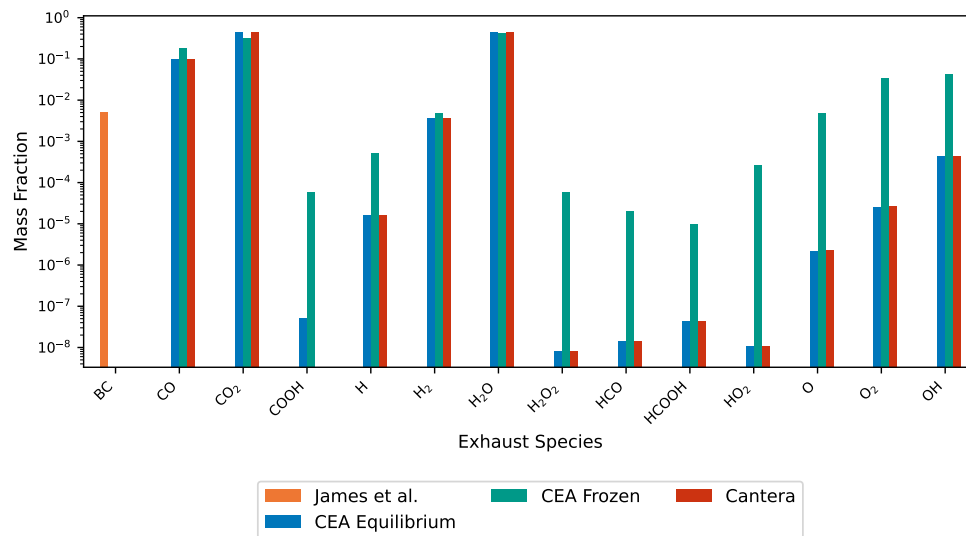


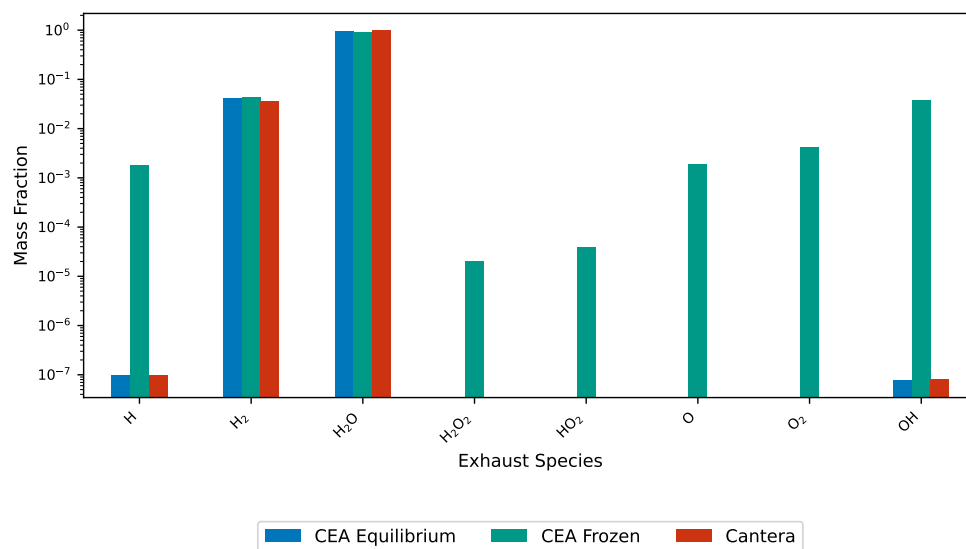
Figure S4. Schematic overview of the CEA and Cantera calculation logic. Rectangles represent programmes, trapezoids represent input-outputs, and diamonds represent decisions. Input parameters are shown in red, external software implemented is shown in blue. NRLMSIS is an atmospheric model, CEA and Cantera are combustion models. Mass profile and emission index could also be implemented directly by the user. Details are explained in the text.

55 S2.3 Exhaust evaluation

For the exhaust calculation the specific engine and propellant parameters for the Merlin engine (LOX/RP-1), Raptor engine (LOX/LCH4), Vulcain 2.1 engine (LOX/LH2) and P120 rocket motor (HTPB/Al/APN) were taken into account and calculated for the different methodologies at nozzle level exit. For Merlin and Vulcain 2.1 an additional parallel gas generator combustion were taken into account. Parameters can be found in the supplementary material within the engine worksheet in the LV-Database-file.



(a) Starship Raptor engine exhaust



(b) Ariane 6 Vulcain 2.1 exhaust

Figure S5. Exhaust at engine level of a) a Starship Raptor engine and b) an Ariane 6 Vulcain 2.1 exhaust shown for CEA equilibrium and frozen calculation methodologies in logarithmic scale. Species with a massfraction less than $1e-10$ are not shown. A higher variety of species can be seen for the equilibrium methodology for solid engines and frozen methodology for liquid engines. CEA equilibrium and Cantera showing consistency of results. For Vulcain 2.1 an additional gas generator was considered, which leads to slightly more H_2 emissions compared to Cantera. James et al. (2021). BC estimation showing a consistency with additional calculation. CEA frozen calculation leads to more species.

60 S2.4 Emission evaluation

For the emission profiles the x_{ab} was deviated between 1.2, 2, 4 and 8. This should cover an reasonable area based on expert judgement. A further discussion on this uncertainty impact will be given in the second part of the paper.

S2.4.1 Falcon 9

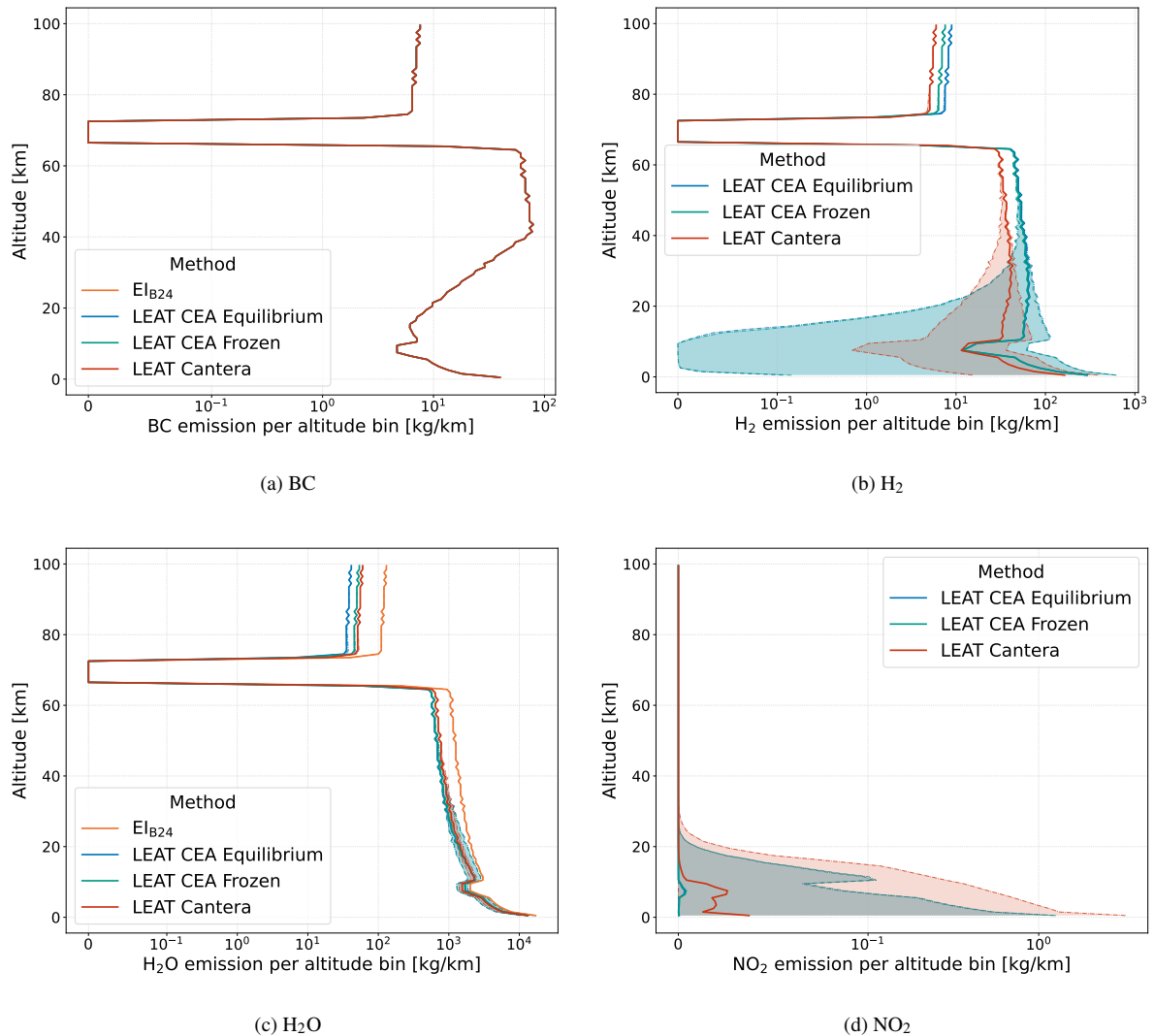
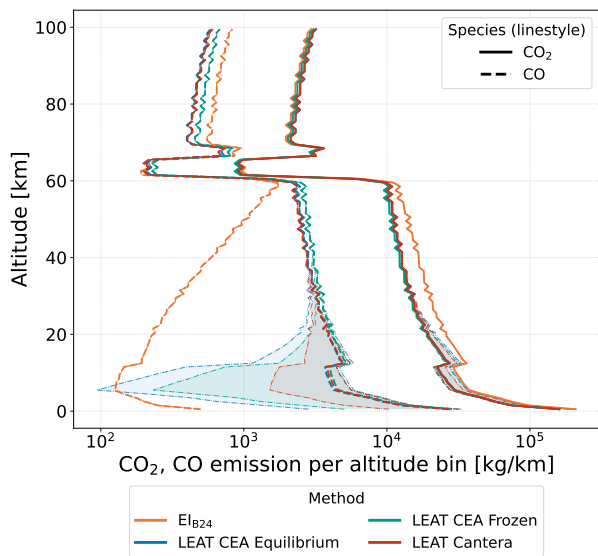
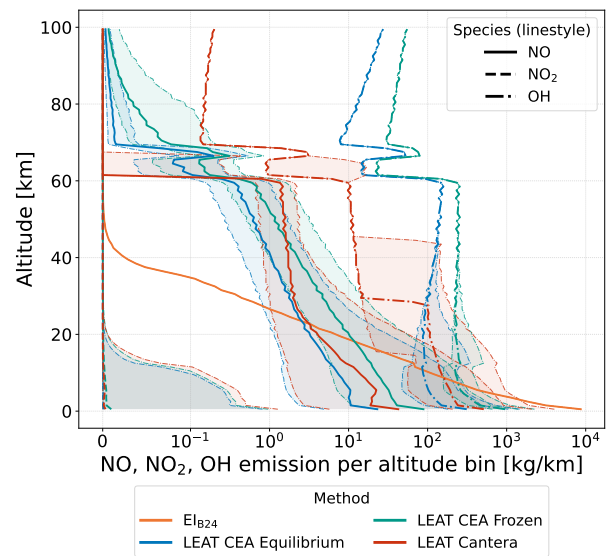


Figure S6. Final emission of Falcon 9 launch depending on altitude shown for different calculation methodologies. Area represents $x_{ab} = 1.2 - 8$, line represents $x_{ab} = 2$.

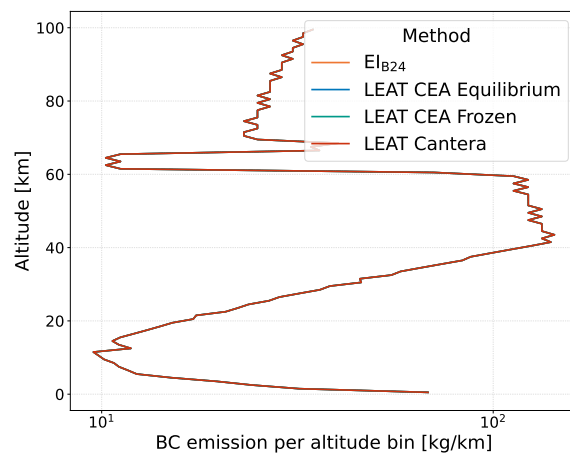
S2.4.2 Starship



(a) CO₂ and CO



(b) NO, NO₂ and OH



(c) BC

Figure S6. Final emission of Starship IFT8 launch depending on altitude shown for different calculation methodologies. Area represents $x_{ab} = 1.2 - 8$, line represents $x_{ab} = 2$.

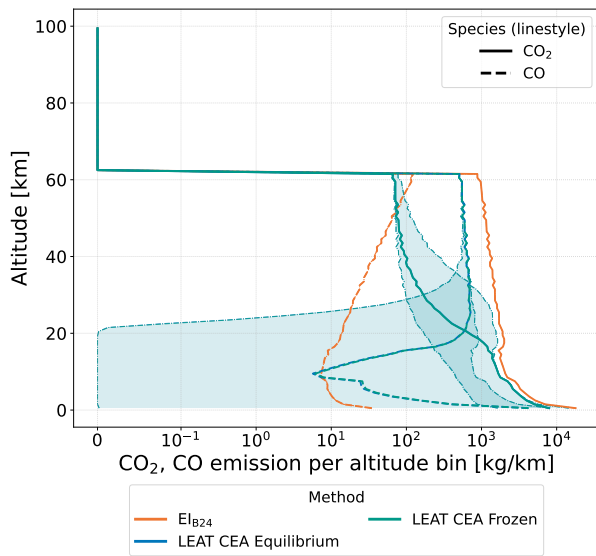
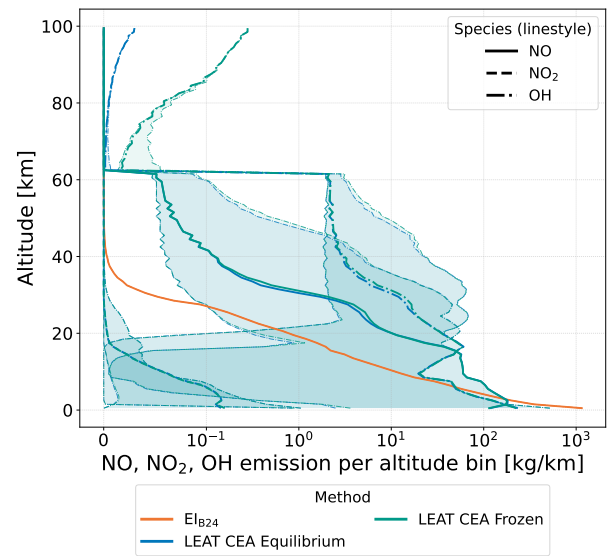
(a) CO₂ and CO(b) NO, NO₂ and OH

Figure S7. Final emission of Ariane 6 launch depending on altitude shown for different calculation methodologies. Area represents $x_{ab} = 1.2 - 8$, line represents $x_{ab} = 2$.

S3 Input parameters

The Tab. S16 contains all inputs needed to define the launch scenario and launch vehicle.

Table S16: Input parameters of LEAT

Parameter	Description	Format	Unit
launch_sites.xlsx	Geographic data of launch sites		
launch_site	Name for launch site	string	-
lat	Latitude of launch pad	float	°
lon	Longitude of launch pad	float	°
alt	Altitude of launch pad	float	m
scenarios.xlsx	Launch specific data		
scenario	Name for scenario	string	-
launch_vehicle	Name of launch vehicle from launch vehicle database	string	-
date	Date of launch	datetime	YYYY-MM-DD HH:MM:SS T
launch_site	Name of launch site from launch sites file	string	-
azimuth	Azimuth of launch	float	°
payload_mass	Mass of payload	float	kg
h_gt_start	Altitude of start of gravity turn	float	m
h_gt_end	Altitude of end of gravity turn	float	m
gamma_gt_total	Change of gamma of gravity turn	float	°
t_startup	Time of startup till full thrust	float	m
t_fr_start	Time of start of thrust reduction	float	s
t_fr_end	Time of end of thrust reduction	float	s
force_reduced	Amount of thrust reduction	float	-
LV_Database.xlsx/ LV_Database sheet	Launch vehicle data		
LV_Type	Name of the launch vehicle	string	-
l	Total length	float	m
d	Main diameter of rocket	float	m
l_n	Length of nose	float	m
d_n	Diameter of nose	float	m
d_f	Diameter of fairing	float	m
A_e/A_R	Ratio of engine area to reference cross sectional area	float	-
A_R	Reference cross sectional area	float	m
start_with_booster	If booster and first stage are ignited together	boolean	-
stageX_engine	Name of stage engine from engine datasheet	string	-
stageX_force_sl	Thrust of stage at sea level	float	N
stageX_force_vac	Thrust of stage in vacuum	float	N

Continued on next page

Parameter	Description	Format	Unit
stageX_fuel	Name of stage oxidizer and fuel	string	-
stageX_fuel_temp	Temperature of stage propellants	float	K
stageX_total_propellant	Total mass of stage propellant	float	kg
stageX_propellant_massfractions	Massfraction of stage propellants	float	-
stageX_mass_fuel	Total mass of stage fuel	float	kg
stageX_mass_ox	Total mass of stage oxidizer	float	kg
stageX_dry_mass	Total mass of stage drymass	float	kg
stageX_burntime	Burning time of stage	float	s
<hr/>			
LV_Database.xlsx/ Engine sheet	Launch vehicle engine data		
<hr/>			
engine	Name of engine	string	-
Ae/At	Nozzle area expansion ratio	float	-
p_chamber	Pressure of combustion chamber	float	bar
engine_cycle	Type of engine cycle (GG = Gasgenerator)	float	-
mf_oc	Share of massflux threw gas generator	float	m
rof_oc	Ratio of oxidizer to fuel for gas generator	string	-
Ae/At_oc	Nozzle expansion ratio of gas generator	float	-
p_chamber_oc	Pressure in the combustion chamber of the gas generator	float	bar

S4 Configuration parameters

The Tab. S17 contains the configurations that could be made when using the tool.

Table S17: Configuration parameters of LEAT
























Parameter	Description	Format	Unit
General Config		Configurations for calculations	
all_scenarios	When False only the user_defined_scenarios will be processed	boolean	-
user_defined_scenarios	Scenarios to be calculated if all_scenarios = False	array of strings	-
use_external_trajectory_data	Trajectory for input for one scenario	boolean	-
file_name_ext_trajectory	File name of external trajectory	string	-
Trajectory Config		Trajectory calculation configuration	
t_max	Maximum simulation time	integer	s
numeric_method	Numerical calculation method to be used ('RK45', 'RK23', 'DOP853', 'BDF')	string	-
max_step	Step size	float	s
atol	Absolute tolerance	integer	-
rtol	Relative tolerance	integer	-
use_ode_break	Choose if you want to include an ODE Break Event based on height	boolean	-
height_ode_break	Maximum Simulation Height	integer	m
v_0	Initial state: Speed without earth rotation	integer	m/s
x_0	Initial state: Horizontal distance	integer	m
s_0	Initial state: Total distance	integer	m
gamma_0	Path angle relative to horizon initially at 90° (vertical start)	integer	°
compress_data	Compress trajectory data	boolean	-
compress_method	Choose between "time" or "height" as the compression interval	string	-
compress_interval	Choose interval steps	integer	s or m
compress_atmosphere	Choose "averages" to average the atmosphere data of the interval Or choose "latest" for just the value at the given time/height step	string	-
interval_tolerance	Allow for floating-point precision issues	float	-
Emissions Config		Emission calculation configuration	
calculate_emissions	Choose if you want to include emission calculation to trajectory calculation	boolean	-
use_emission_factors	Calculation with emission indices	boolean	-
emission_factor_method	Calculation methodology of emission indices (stoichiometric, LEAT, Barker2024_seco, Brown2024, James2021, Larson2017, Pradon2023, Ross2009, Ross2014, Ryan2022, or own added values)	string	-
use_nasa_cea	Calculation with NASA CEA	boolean	-
use_cantera	Calculation with Cantera	boolean	-
calculate_black_carbon	Additional BC calculation according to James et al. 2021	boolean	-

Continued on next page

Parameter	Description	Format	Unit
threshold	Threshold for species to be considered not zero	float	-
trace	Value until CEA considers trace gases	float	-
rocket_equilibrium	Use equilibrium for CEA calculation	boolean	-
rocket_frozen	Use frozen for CEA calculation	boolean	-
frozen_nfz	Defines the point of reaction freezing (1 = combustion chamber, 2 = throat, 3 = exit)	integer	-
frozen_nfz_exception_fuels	Defines the propellants for which the exception freezing point is taken into account	array of strings	-
frozen_nfz_exception	Defines the point of reaction freezing for exception fuels	integer	-
afterburning	Include afterburning calculation	boolean	-
problem_afterburning	Defines the mode of afterburning (tp, hp & uv)	string	-
x_ab	Afterburning uncertainty factor	float	-

70 S5 File structure

LEAT

 <code>input_data/</code>	Contains all input files
 <code>cea_species.yaml</code>	Thermodynamic database of CEA for Cantera
 <code>config.py</code>	Configurations of program
 <code>emission_factors.xlsx</code>	Emission indices database
 <code>launch_sites.xlsx</code>	Launch sites database
 <code>LV_Database.xlsx</code>	Launch vehicle database
 <code>scenarios.xlsx</code>	Scenarios database
 <code>trajectory_results_cleaned.csv</code>	Input trajectory example
 <code>NASA_CEA/</code>	NASA CEA tool and related files
 <code>output_data/</code>	Folder for storing output results
 <code>data_raw/</code>	Raw output files
 <code>emissions/</code>	Emission results
 <code>trajectory/</code>	Trajectory and atmospheric data
 <code>plot_emission.py</code>	Plots emission in altitude bars
 <code>scripts/</code>	Helper scripts
 <code>data_processing.py</code>	Handles data inputs and outputs
 <code>emissions.py</code>	Emission calculation script
 <code>trajectory.py</code>	Trajectory calculation script
 <code>cleanup_output_data.py</code>	Script to clear output data
 <code>LICENSE.txt</code>	Software License Agreement
 <code>main.py</code>	Main entry point for the tool
 <code>README.md</code>	Main README
 <code>requirements.txt</code>	Required Python Modules

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