Appendix G.
Exhaust Plume Calculations

Sierra Engineering & Software, Inc.

ANALYSIS REPORT

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SUBJECT: Exhaust Plume Calculations for SpaceX Raptor Booster Engine

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PREPARED FOR: SpaceX
(W.O. 6017)

1.0 SUMMARY

Calculations were performed to estimate the far-field exhaust constituents of the SpaceX Raptor2 liquid oxygen-liquid methane (LOX-LCH4) booster rocket engine firing under sea-level conditions. Although the exit-plane exhaust is fuel-rich and contains high concentrations of carbon monoxide (CO), subsequent entrainment of ambient air results in nearly complete conversion of the CO into carbon dioxide (CO_2). A small amount of nitrous oxide (NO) also formed in the combustion chamber as a result of N2 present in the propellants. There is some burnout of the NO during the plume entrainment process. More importantly, the rapid mixing of ambient air into the Raptor2 plume minimizes the formation of thermal NO_x. The CO and NO emissions are predicted to be 2.59 lb_m/s and 5.62 lb_m/s respectively, per engine, under nominal power (100%) operation. No soot is predicted to be generated by this engine cycle. The Super Heavy booster emission rates have been estimated to be 85.6 and 185.5 lb_m/s for CO and NO, respectively. CO_2 emissions from a single engine and a Super Heavy booster are 1202.5 and 39,681 lb_m/s, respectively.

2.0 ENGINE DESCRIPTION

The subject engine is the upscaled booster engine for the SpaceX Super Heavy launch vehicle. The baseline Super Heavy stage includes 33 Raptor2 engines. The propellants are liquid oxygen (LOX) and liquid methane (LCH4). Unlike previous analyses, these analyses include approximately 0.5% nitrogen in both the fuel and oxidizer to simulate real propellant characteristics. The subject engine uses a closed power cycle with a regeneratively-cooled thrust chamber nozzle. Characteristic nozzle exit radius is included in Table 1.

The current analysis was performed for the 100% nominal engine operating condition, with model results matched test performance data.

Table 1: Raptor2 Nozzle Characteristics

Nozzle exit radius Rj (in)	25.718

3.0 ANALYSIS APPROACH

A series of simulations were required to estimate the emissions from the Raptor2 engine. The PERCORP analysis model[1] was used to estimate the O/F mixture ratio variations that exist within the Raptor2 thrust chamber. The VIPER parabolized Navier-Stokes model[2] was used to kinetically expand the thrust chamber exhaust to the nozzle exit plane. The VIPER results were used to assess the validity of the PERCORP solution, correlating engine thrust, mass flow rate and specific impulse (ISP) to test results. PERCORP input parameters were adjusted until there was good agreement between the VIPER performance predictions and the test results. The SPF code[3] was used to predict the flow structure of the free exhaust plume and the entrainment of ambient air. VIPER solution was used as the inflow starting condition for the SPF. Though the SPF code can handle detailed chemical kinetics within the evolving plume flow field, the strong barrel shock downstream of the nozzle exit produces numerical convergence problems with the version of SPF used. The present SPF simulations were performed without chemical kinetics. The SPF results were air entrainment and gas temperature profiles. The SPF and VIPER results were used as inputs for one-dimensional kinetic modelling of the plume flow field. The kinetic model in the TDK code[4] was used to model chemical reactions within the evolving plume flow field.

TDK modelling of the plume flow field included chemical mechanism that address

a) the oxidation of CO to CO_2,

b) the complex oxidation of hydrocarbons to H_2O and CO_2, and

c) the thermal generation and destruction of NOx in a mixture of air and combustion products.

Table 2 includes the chemical reactions and rates used in the TDK simulation.

Table 2: Kinetic Reactions Included in One Dimensional Chemistry Simulations[*]

	A	N	B
H + H + m = H2 + m[†]	6.4E17	1.0	0.0
H + OH + m = H2O + m	8.4E21	2.0	0.0
O + O + m = O2 + m	1.9E13	0.0	-1.79
CO + O + m = CO2 + m	1.0E14	0.0	0.0
O + H + m = OH + m	3.62E18	1.0	0.0
CH4 + m = CH3 + H + m	1.259E17	0	88.4
HCO + m = CO + H + m	5.012E14	0	19.0
C2H3 + m = C2H2 + H + m	7.943E14	0	31.5
N+NO = N2+O	2.700E13	0	0.355
N+O2 = NO+O	9.000E9	-1.0	6.5
N+OH = NO+H	3.360E13	0	0.385
HO2+NO = NO2+OH	2.110E12	0	-0.480
NO2+O = NO+O2	3.900E12	0	-0.240
NO2+H = NO+OH	1.320E14	0	0.360
O2 + H = O + OH	2.2E14	0.0	16.8
H2 + O = H + OH	1.8E10	-1.	8.9
H2 + OH = H2O + H	2.2E13	0.0	5.15
OH + OH = H2O + O	6.3E12	0.0	1.09
CO + OH = CO2 + H	1.5E7	-1.3	-.765
CO + O = CO2	2.5E6	0.0	3.18
CO2 + O = CO + O2	1.7E13	0.0	52.7
CH4+ OH = CH3 + H2O	3.162E13	0	6.0
H + CH4 = CH3 + H2	6.310E14	0	15.1
O + CH4 = CH3 + OH	3.981E14	0	14.0
CH3 + O = CH2O + H	1.259E14	0	2.0
CH3 + OH = CH2O + H2	3.981E12	0	0
C2H2 + OH = C2H + H2O	6.310E12	0	7.0
H + CH2O = HCO + H2	3.162E14	0	10.5
O + CH2O = HCO + OH	1.995E13	0	3.1

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[*] TDK reaction format is k=AT**(-N)*EXP(-1000B/RT) [cc-Kcal-K-mole-s]

[†] m is any molecule for a third body reaction

Table 2: Kinetic Reactions Included in One Dimensional Chemistry Simulations (ctd)

	A	**N**	**B**
OH + CH2O = HCO + H2O	7.943E12	0	0.2
H + HCO = CO + H2	1.995E14	0	0
OH + HCO = CO + H2O	1.000E14	0	0
H + C2H2 = C2H + H2	1.995E14	0	19.0
O + C2H2 = CH2 + CO	5.012E13	0	3.7
C2H + O2 = HCO + CO	1.000E13	0	7.0
CH2 + O2 = HCO + OH	1.000E14	0	3.7
H + C2H4 = C2H3 + H2	1.000E14	0	8.5
C2H2 + H = C2H3	5.500E12	0	2.39
H + C3H6 = C2H4 + CH3	3.981E12	0	0

4.0 ANALYSIS RESULTS

The PERCORP modelling of the Raptor2 thrust chamber included film coolant. The PERCORP solution for the nominal engine specific impulse includes a core mixing loss, yielding a characteristic velocity (C*) efficiency that is consistent with test results. The PERCORP results included initial boundary conditions for the VIPER nozzle flow field simulation. The predicted thrust chamber nozzle exit species mass fractions from VIPER are listed in Table 3.

The SPF modelling stepped to 150 nozzle exit radii (Rexit = 25.718 inches, 2.143 ft). Since the propellants contain N2 for the current simulations, the air was modelled as a more complex N2-O2-Ar-CO2 mixture (0.7807/0.2095/0.00934/0.000412 moles fraction).[5] This approach allowed the Ar to serve as a marker for air entrainment. Predicted plume contours for temperature and mass fractions of argon (Ar), CO and NO are presented in Figure 1 through Figure 4. Since there plume entrainment and mixing field is simulated for chemically frozen flow, the Ar contours are representative of the air entrainment, while the CO and NO contour indicates a key product of incomplete combustion that were created by the engine.

Table 3: Thrust Chamber Nozzle Exit Species Mass Fraction from VIPER Simulation

Species	Mass Fraction
CO2	0.4118
H2O	0.4147
CO	0.1114
O2	0.0428
H2	0.0071
OH	0.0035
O	0.0004
CH4	0.0001
H	0.00004
NO	0.0037
NH3	0.000009

Figure 1: Air Entrainment Plume Temperature Contours (degrees K)
R/Rj and X/Rj are Normalized by the Nozzle Exit Radius Rj

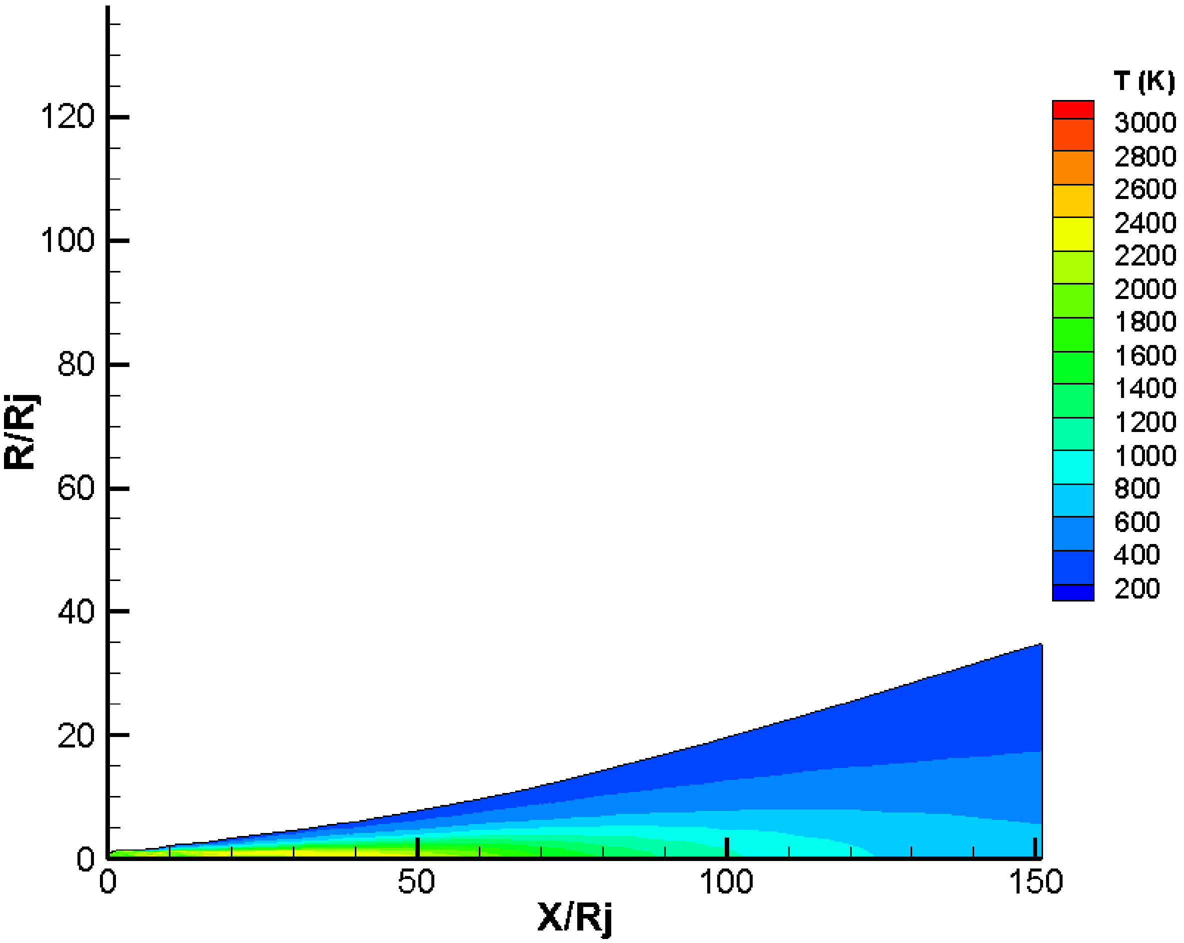


Figure 2: Plume Ar Mole Fraction Contours
R/Rj and X/Rj are Normalized by the Nozzle Exit Radius Rj

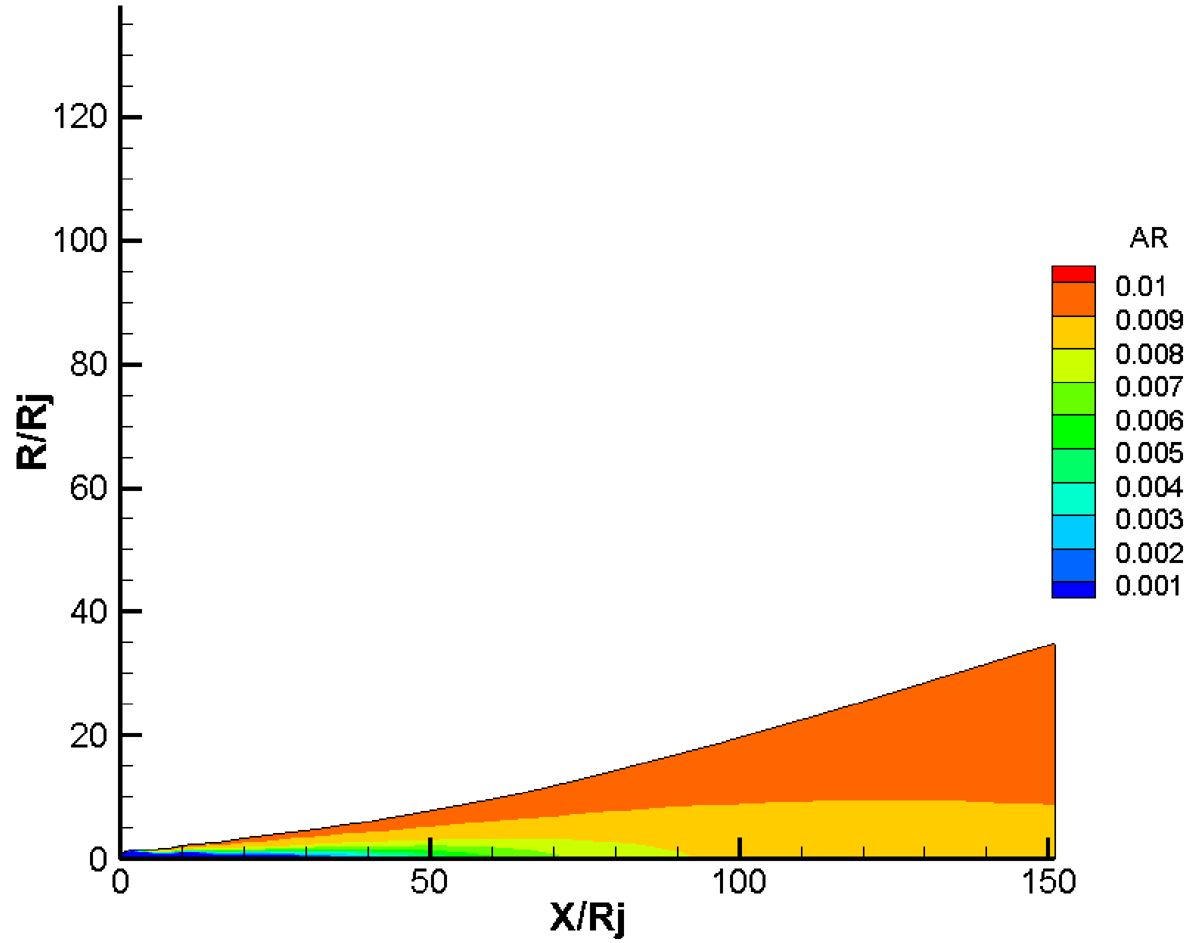


Figure 3: Non-Reacting Plume CO Mole Fraction
R/Rj and X/Rj are Normalized by the Nozzle Exit Radius Rj

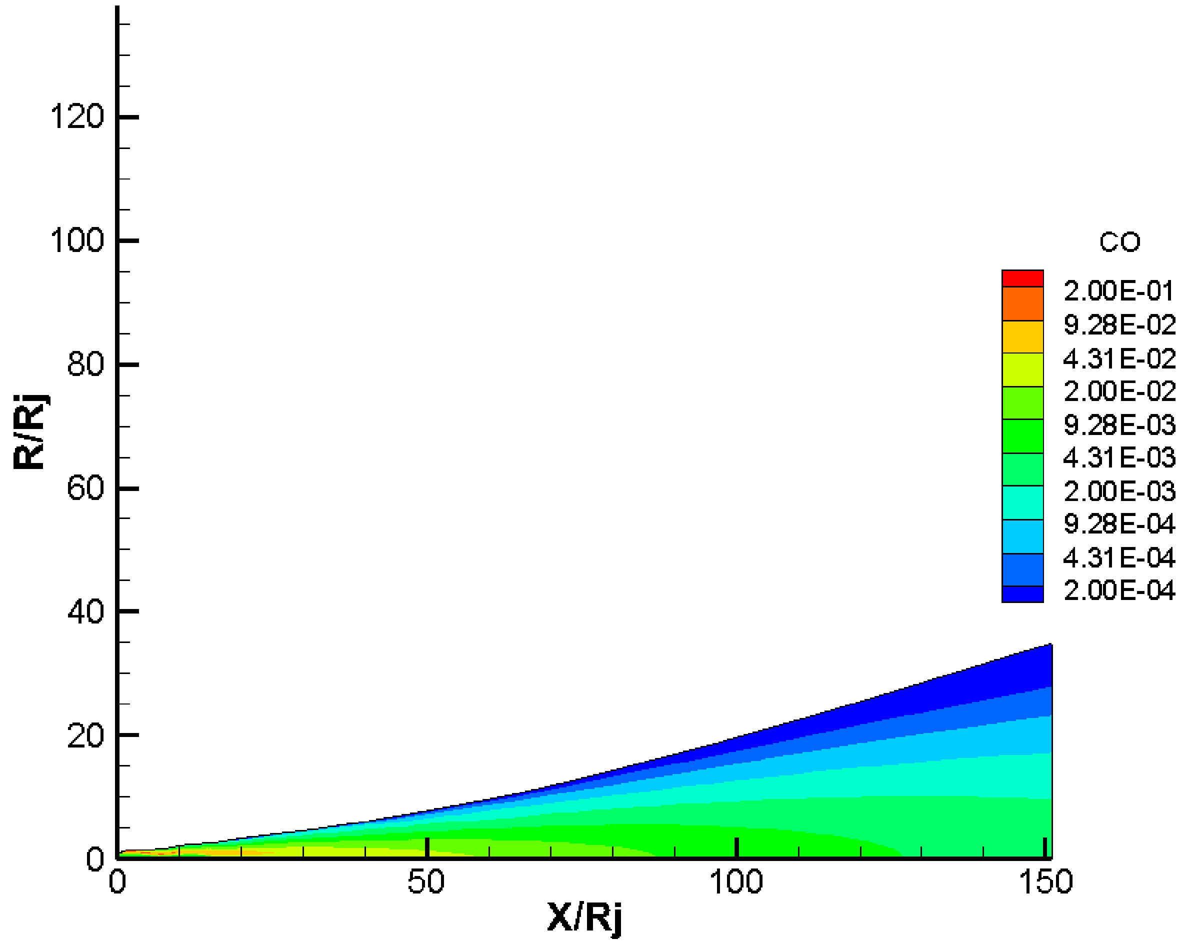
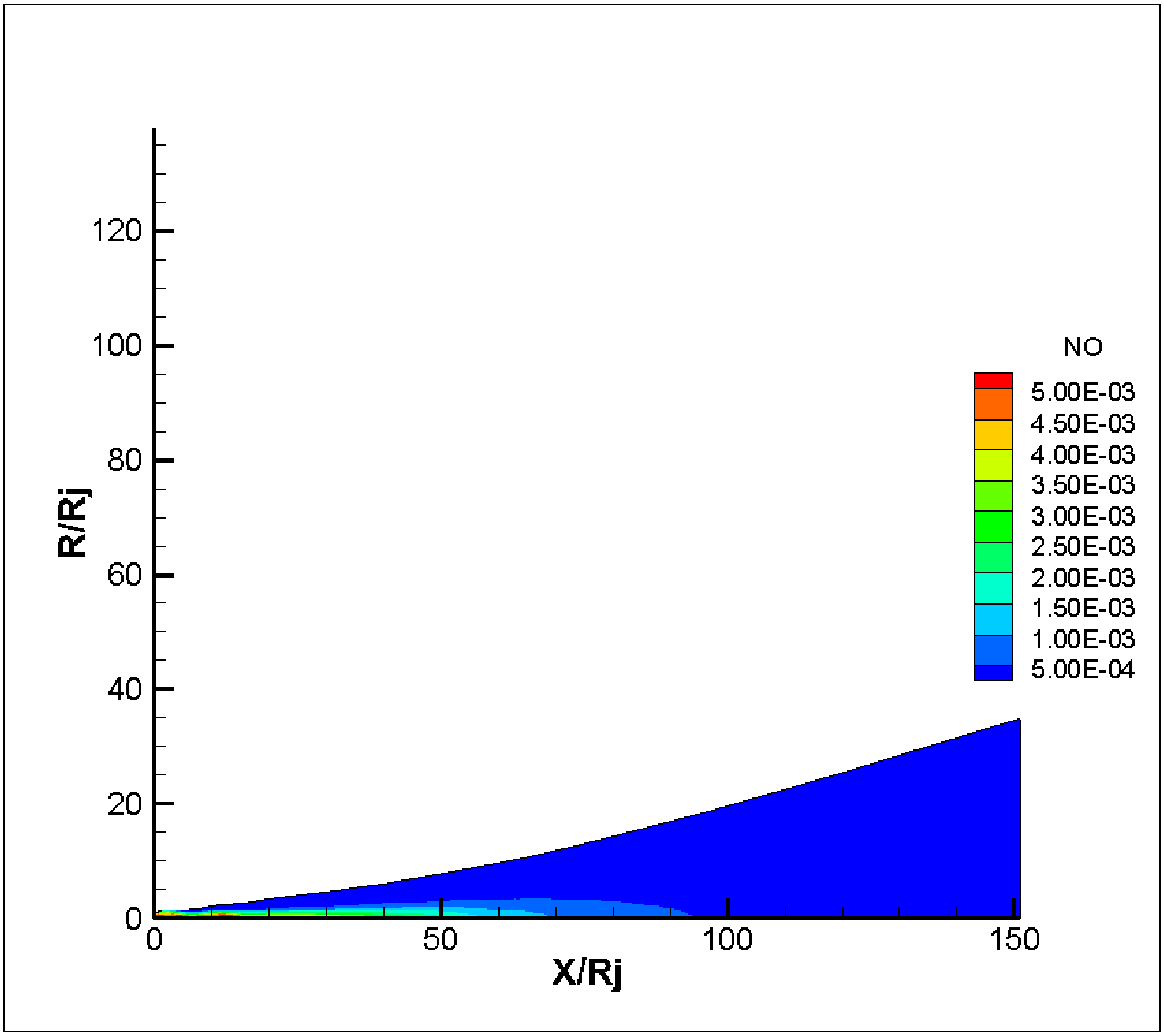


Figure 4: Non-Reacting Plume NO Mole Fraction
R/Rj and X/Rj are Normalized by the Nozzle Exit Radius Rj



Integration of the SPF data indicates that 430,783 lbm/s air is entrained by the core jet is indistinct (Figure 5). It is estimated that the 215-foot jet end point is reached 433 msec after the plume flow exits the nozzle.

The subsequent TDK simulation of the plume chemistry required an approximate fit of the air entrainment rate. The SPF air entrainment profile was fit to an “availability profile” for the TDK simulations, whereby ambient air is mixed into the plume flow. Figure 6 shows that the approximate TDK air addition agrees well with the entrainment rate predicted by SPF.

Figure 5: Axial Air Entrainment Estimates from SPF.

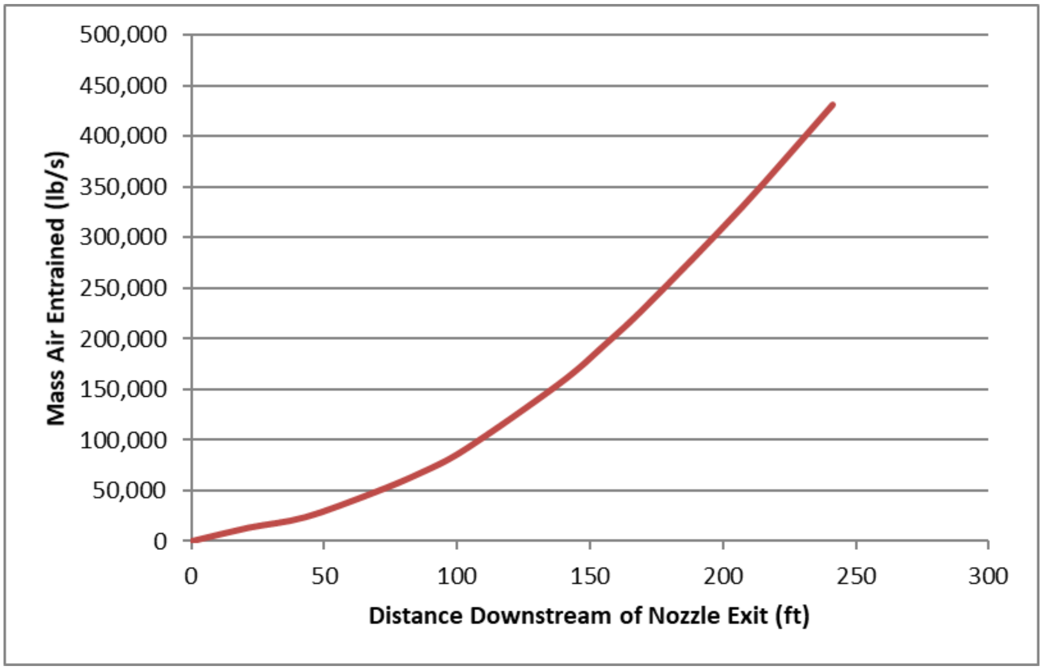
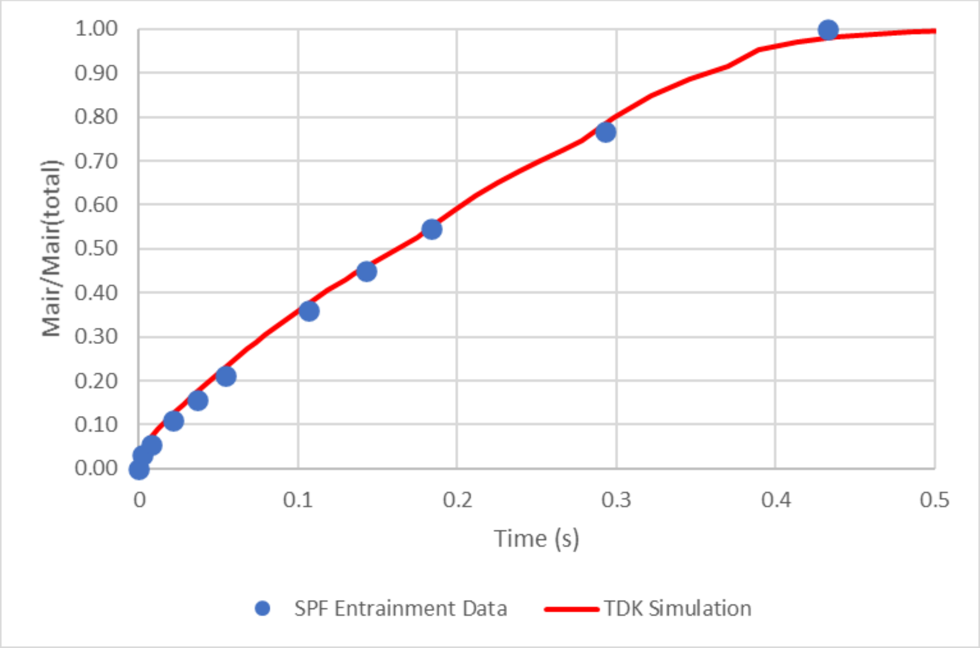
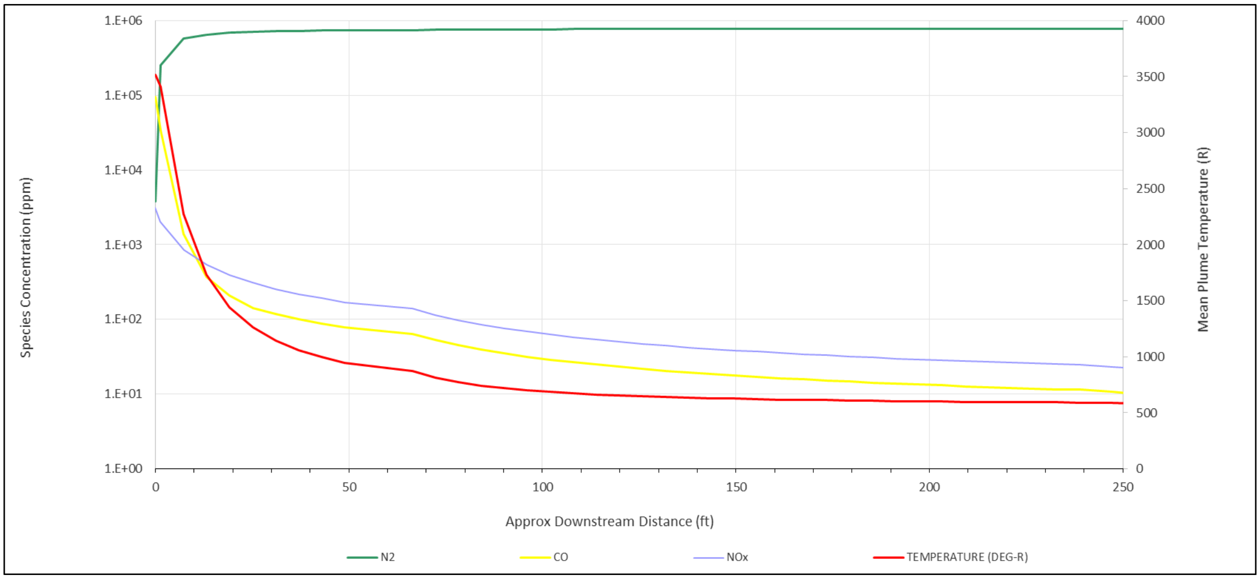


Figure 6: Approximate Air Entrainment Profile used in TDK Simulations



The one-dimensional kinetics modeling of the after-burning characteristics of the exhaust plume was performed assuming a piecemeal constant pressure (13.3-14.7 psia) and entrainment of ambient temperature air. The underexpanded nature of the Raptor2 nozzle exit flow induces rapid entrainment of ambient air into the plume, dropping the exhaust temperature and freezing kinetically controlled reactions. The small concentration of unburnt methane is rapidly oxidized, surviving less than 1 msec. The model predicted that nearly complete CO oxidation occurs, with concentrations reduced to 6 ppm at the end of plume simulation. The plume exit concentration is approximately 95,400 ppm (9.54%). There is no significant thermal NO formation in the plume, but the presence of N2 in the propellants produces 3115 ppm NO in the main combustion chamber. The NO mole fraction at the end of the 240 ft long plume entrainment is 13 ppm. Given the total mixed plume mass flow rate of 432,386 lb/s, this corresponds to 5.62 lb_m/s for NO and 2.59 lbm/s CO. Figure 7 shows the predicted temperature and pollutant species concentration profiles. The total CO_2 emission from the plume entrainment is 1202.5 lb_m/s. The pollutant flow rates were calculated in terms of lb_m generated per second of steady engine operation.

Figure 7: Predicted Profile of Bulk Plume Temperature and Species Mass Fraction



Due to the complexity of how the 33 engines are integrated into the base of the Super Heavy vehicle, there is not a simplified method to directly predict the air entrainment and exhaust burnout chemistry for the installed engines. An extensive computational fluid dynamics (CFD) analysis would likely be needed to fully address the entrainment process. However, engineering judgement can be used bound the problem. The outermost 20 engines will entrain air like the single engine for the outboard portion of their flow (about 50%), but the inboard portion of the flow will interact with the exhaust from the inner engines, delaying the time and distance before the plume flow field interacts with ambient air. The centermost 13 engines will likely entrain rocket exhaust plume for a significant amount of time before air entrainment begins. The effluent from the rocket nozzle exhaust primarily contains both CO and NO as unburned combustion products. The single engine analysis shows the rapid air entrainment cools the plume before significant thermal NO formation can occur. It is likely that the hot interior and CO and NO will oxidize as soon as air is available (entrained), though there may be a small time window when the exhaust is hot and there is air introduced, allowing formation of thermal NOx. With this description of the global flow field generated by the Super Heavy, it is likely that the exhaust plume length is 3-4 times longer than predicted for a single engine (720-960 ft), but that the CO, NO and CO_2 emission for the Super Heavy should be about 33 times the single engine level (85.6, 185.5 and 39,681 lb_m/s for CO, NO and CO_2, respectively).

5.0 REFERENCES

[1] *Performance Correlation Program (PERCORP) Reference and User's Manual, Version 3.1.1,* Sierra Engineering & Software, Inc., Sacramento, CA, March 2022

[2] *Viscous Interaction Performance Evaluation Routine For Two-Phase Nozzle Flows With Finite Rate Chemistry, VIPER 5.0*, Software and Engineering Associates, Carson City, NV, 2021

[3] Taylor, M.W. and Pergament, H.S.; *Standardized Plume Flowfield Model SPF-III, Version 4.2 Program User's Manual*, PST TR-51, Propulsion Science and Technology, Inc. East Windsor, NJ, June 2000

[4] Nickerson, G. R., Dunn, S.S., Coats, D.E. and Berker, D.R.; *Two-Dimensional Kinetics (TDK) Nozzle Performance Computer Program User's Manual*, Software and Engineering Associates, Carson City, NV, Jan 1999

[5] https://www.engineeringtoolbox.com/air-composition-d_212.html#Table, viewed 24 March 2022